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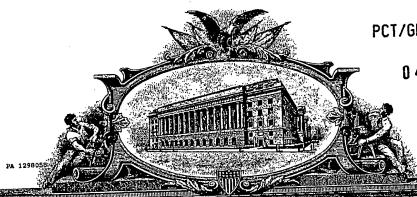
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### PROVISIONAL APPLICATION FOR PATENT COVER SHEET

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#### RECEPTOR MODULATORS

#### Field of the Invention

The present invention relates to use of a crystal structure to obtain modulators of a cell surface receptor and to the generation of therapeutic antibodies and chimeric proteins that bind a particular class of signalling receptors.

#### Background of the Invention

CD28 is present on the surface of T cells and plays an important role in their activation. Signal transduction occurs through CD28 after it is activated (triggered) by binding to its ligand. CD28 activation is dependent on phosphorylation of its cytoplasmic domain. CD28 does not have intrinsic phosphorylation activity but instead is dependent on an extrinsic kinase, e.g. p56lck.

#### Summary of the Invention

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The invention relates to the obtaining of the structure of CD28. This was done by crystallizing a CD28/Fab fragment complex, subjecting it to X-ray diffraction and deriving the structural coordinates from the diffraction measurements. The Fab fragment is from an antibody that has superagonist activity towards CD28, i.e. is able to cause activation of CD28 without the need for a T cell receptor-derived signal. Conventional antibodies that activate CD28 need an additional signal generated by the T cell receptor. The deduced structure allows modulators of CD28 signalling to be obtained which can in turn be used to modulate the immune system.

Accordingly the invention provides a method of identifying a modulator of CD28 comprising comparing a structural model of a candidate modulator with a structural model of CD28 to thereby determine whether the modulator will bind to CD28, wherein the structural model is derived from, or comprises, structural coordinates of a crystal of: (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii).

In addition the invention relates to antibodies and chimeric proteins that are capable of being superagonists of particular receptors by preferentially excluding phosphatases (as opposed to kinases) from the vicinity of the said receptor.

Accordingly the invention provides an antibody that causes superagonistic signalling of a cell surface receptor, wherein said antibody binds to the extracellular portion of the receptor at a membrane proximal region and said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase, wherein said antibody does not bind only the C'-D loop of human CD28.

In addition the invention provides a chimeric protein that causes superagonistic signalling of a cell surface receptor, which chimeric protein comprises (i) sequence representing a fragment of a ligand of the receptor, or a homologue of such a fragment, wherein the fragment or homologue is capable of binding to the extracellular portion of the receptor at a membrane proximal region, and (ii) an Fc region of an antibody, wherein said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase.

Further the invention provides a chimeric protein that causes superagonistic signalling of a first cell surface receptor, which chimeric protein comprises two Fv regions of an antibody that may be the same or different, wherein at least one of the Fv regions is capable of binding to said first receptor, and the other Fv region binds to a second cell surface receptor expressed on another cell, wherein said first receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase, and the first receptor can be identical to the second receptor.

#### Description of the drawings

Figure 1 shows mechanisms of differential triggering of extrinsic kinasedependent receptors, by superagonistic agents in vitro and in vivo.

A. In vitro superagonistic signalling, giving the example of CD28 antibodies. The basic signalling principle is as follows. Antibodies raised against CD28 bind distally ("conventional" antibodies, left) or membrane-proximally ("superagonists", right), as indicated by the structure of the CD28-5.11A1 antibody-Fab complex. The antibodies hold the cell surface at certain distances from an immobilising substrate: in this case plastic, and as shown in parts B, C and D of the figure, Fc receptor-or other receptor-bearing cells. For superagonistic antibodies this distance is typically 150-200Å, whereas for costimulatory antibodies, it is considerably larger.

The induced proximity of the membrane and the immobilising substrate in the region of the immobilised antibody and receptor will lead to the differential steric exclusion, from the immediate vicinity of the receptor, of other molecules whose extracellular domains are comparable in size or larger than CD28-antibody complexes, such as the tyrosine phosphatase, CD45. In contrast, tyrosine kinases, e.g. p56lck, will be unaffected because they are small and/or attached to the inner leaflet of the membrane. The result is that, overall, the phosphorylation of CD28 by the kinases will be favoured over its de-phoshorylation by phosphatases, with the net increase in phosphorylation amounting to receptor triggering. Superagonists are more potent than conventional antibodies because they bind epitopes close to the membrane rather than at the "top" of the molecule, leading to more efficient exclusion of, e.g., CD45, and therefore a larger increase in the net phosphorylation of CD28.

B. In vivo superagonistic signalling, giving the example of CD28 antibodies. The binding of the antibody to the membrane-proximal region of CD28 on a T cell, and to the Fc receptor of, e.g. an antigen presenting cell, forces the membranes of the two cells into close proximity (150-200 Å). This in turn excludes CD45 from the immediate vicinity of CD28 as described in A, leading to signalling by CD28.

C. In vivo superagonistic signalling, giving the example of a chimeric, ligand-based agent. The chimera consists of a receptor-binding region of the ligand of the receptor, fused to the Fc region of an antibody. The binding of the ligand portion of the chimera to the receptor, and of the Fc region of the chimera to the Fc receptor of, e.g. an antigen presenting cell, forces the membranes of the two cells into close proximity (150-200 Å). This in turn excludes CD45 from the immediate vicinity of the receptor as described in A, leading to signalling by the receptor.

D. In vivo superagonistic signalling, giving the example of a chimeric, Fv-based agent. The chimera consists of the receptor-binding Fv region of one antibody, fused to the Fv region of a second antibody reactive with another receptor on a second cell. The binding of the chimera to both receptors forces the membranes of the two cells into close proximity (150-200 Å). This in turn excludes CD45 from the immediate vicinity of the receptor as described in A, leading to signalling by the receptor.

Figure 2 shows the method for identification of binding sites for superagonist antibodies of receptors raised against example receptors.

#### Description of the sequences mentioned herein

SEQ ID NO:1 shows the amino acid sequence of CD28.

SEQ ID NO:2 shows the sequence of the CD28/Fc fusion protein used to express and dimerise CD28.

#### Detailed description of the invention

The CD28 protein

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Many of the different aspects of the invention discussed herein refer to CD28. It is to be understood that references to CD28 herein also include (i) a homologue of CD28, or (ii) a fragment of CD28 or the homologue, or (iii) a fusion protein comprising CD28, (i) or (ii), unless the context requires otherwise. The homologue and/or fragment of CD28 may be of particular lengths, as discussed below, or may have the binding or functional properties of naturally occurring (native) CD28, such as the ability to bind a cell membrane and/or bind to B7-1 or B7-2. The homologue and/or fragment may comprise the extracellular domain of CD28. The homologue and/or fragment may comprise, or essentially consist of, the fragment of CD28 present in the fusion protein of SEQ ID NO:2. The homologue and/or fragment may have the ability to transduce a signal to the cytoplasm of a T cell.

The CD28 may be of any species of animal, such as a mammalian or avian CD28. The CD28 is preferably a human CD28, for example as shown in SEQ ID NO:1. The CD28 protein may be present in particular forms, for example which aid expression and/or crystallization. Thus the CD28 may be fully glycosylated, partially glycosylated or lack glycosylation and/or have a reduced and alkylated stalk region.

The CD28 crystal

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The crystal of CD28 generally comprises CD28 present in a regular repeating array. As mentioned above the term "CD28" includes fragments and/or homologues. Preferred fragments or homologues present in the crystal comprise the extracellular

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domain of native CD28. In the crystal the CD28 is preferably in the form of a monomer. The crystal may be of CD28 bound to another moiety. Such a moiety may be an antibody specific for CD28, including fragments/ derivatives of the antibody (as further discussed below), which bind CD28. In a preferred embodiment the crystal is of CD28 bound to the Fab fragment of an antibody. The crystal may comprise CD28 in a form that aids crystallization, and thus the CD28 may be fully glycosylated, partially glycosylated or lack glycosylation and/or have a reduced and alkylated stalk region. In one embodiment the crystal has the coordinates shown in Table 4.

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The crystal is generally obtained by providing a solution that comprises CD28 and optionally a moiety that binds to CD28, such as an antibody fragment, and subjecting the solution to conditions that allow the crystal to form. The CD28 which is to be crystallized is generally obtained by recombinant expression, optionally in the form of a fusion protein. The fusion protein may comprise CD28 and a polypeptide sequence which forms a homodimer. Such a fusion protein aids the formation of a CD28 homodimer. Preferably the fusion protein comprises the sequence of the Fc region of an antibody. The fusion protein may be cleaved before crystallisation to separate CD28 from the other polypeptide sequence, for example by thrombin.

The CD28 may be expressed in any suitable cell that is able to express large amounts of CD28, such as a Chinese hamster ovary (CHO) cell.

The CD28 may be further treated in order to aid crystallization. Binding to an antibody fragment, such as a Fab fragment, may be used to prevent the N-linked glycans present on the fully glycosylated form of CD28 from inhibiting the crystallisation of the protein. In one embodiment the antibody (or fragment thereof) is a superagonistic antibody, which may have any of the properties of the superagonistic antibodies mentioned herein. Thus, in one embodiment the antibody (or fragment thereof) binds to a loop region in the extracellular membrane proximal region of CD28, such as the C'-D loop (said loop being defined for example as defined in US-A1-2003/0166860 as the sequence from amino acid positions 52 to 66 CD28 represented by the sequence GNYSQQLQVYSKTGF).

The treatment may comprise reduction of the interchain disulphide bonds in the stalk-like region of CD28, e.g. using dithioreitol (DTT). The reduced cysteines may then be inactivated, for example by alkylation (typically the alkyl moiety has 2 to 6, preferably 2, carbons). The alkylation may be performed using iodoacetamide

Crystallisation is typically carried out at 15 to 25°C, such as at 17 to 19°C, preferably 18°C. Magnesium formate and polyethylene glycol (PEG) may be used as precipitating agents. Preferably precipitation is carried out using 0.15 to 0.25 M magnesium formate (such as 0.2 M magnesium formate) and 15 to 25 % PEG 3350 (such as 20% PEG 3350).

In the work described in the Examples it was found that in order to crystallise CD28 this protein had to be expressed in the form of a fusion protein with a second protein capable of forming a homodimer (the Fc region of an antibody), the fully glycosylated form of CD28 needed to be complexed with an Fab fragment of an antibody in order that the N-linked glycans did not interfere with crystallisation, and the disulphide bonds in the stalk region of CD28 needed to be reduced and alkylated so that the stalk did not interfere with crystallisation. Thus in a preferred embodiment the method of obtaining a crystal of CD28 (including fragment and/or homologue thereof) comprises

- (a) expressing CD28 in the form of a fusion protein with a second protein that is able to form a homodimer, wherein the presence of the second protein in the fusion protein causes CD28 to dimerise,
  - (b) cleaving the second protein from the fusion protein,
- (c) reducing and alkylating the disulphide bond present in the stalk-like region of CD28, and
  - (d) crystallising CD28 bound to the Fab fragment of an antibody.

#### Identifying a modulator of CD28

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The invention provides a method of identifying a modulator using the structural coordinates determined from the above-mentioned crystal of CD28. The structural coordinates used in the method may be in the form of a structural model, such as a three dimensional representation of the structure or a pharmacophore. The coordinates/model typically comprise information relating to the identity of each

atom (i.e. whether it is nitrogen, oxygen, hydrogen etc.) and its three dimensional location (normally defined by three spatial coordinates) in the structure. The model may also comprise additional information relevant to obtaining modulators, such as the electronic charge at different locations in the structure or information concerning whether or not the bonds in the structure can be rotated.

The coordinates/model used in the method typically comprise a specific region of the surface of CD28 corresponding to the site where it is desired for the modulator to bind. Such a site typically comprises Glu-32, Arg-34, Tyr-51, Glu-97, Met-99, Tyr-100, Pro-101, Pro-102, Pro-103, Tyr-104 and Leu-105, or a part thereof which comprises one or more of these amino acids. Preferred modulators bind to such a site or part thereof. In one embodiment the modulator is able to inhibit binding of another moiety to this site. Such a moiety may be an antibody which is specific to the site.

In the method the coordinates/model of CD28 are compared to the structural coordinates/model of a candidate modulator to determine whether or not the candidate modulator will bind to CD28. The comparison may be performed by any suitable means, such as the methods described or referenced in Lyne (2002) Drug Discovery Today 7, 1047-1055. Thus one or more of the algorithms described in this document may be used, such as one or more of Dock, FlexX, FlexE, Slide, Fred, Gold, Glide, AutoDock, LigandFit, ICM, QXP, Amber, CHARMM, SCORE, VALIDATE, Chemscore, Ludi, PLP, PMF, Bleep, SmoG, ZAP, VIDA, GRID, MCSS, Superstar and ROCS.

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The method typically comprises deducing one or more ways of fitting (docking) a candidate modulator with CD28 followed by an evaluation (scoring) of the fit. The evaluation may comprise deducing the binding energy between CD28 and the modulator. This may be done based on the interatomic distances between the atoms involved in binding or by analysis of the force fields of CD28 and the modulator. In one embodiment the evaluation comprises comparing the similarity between the fit between CD28 and the candidate modulator and the fit between one or more other proteins and their ligands. Thus the evaluation may comprise comparison with a database of structures of proteins fitted/bound to ligands.

A candidate modulator which has been selected computationally as discussed above may be physically tested to determine whether or not it is able to bind or modulate CD28. Any suitable binding or activity assay may be used. The binding assay may measure the extent of direct binding between the candidate modulator and CD28 or instead be in the form of a competition assay. The binding assay may comprise/use of any of the following:

- (a) an assay of binding to CD28 (which may be immobilized), for example in which
- (i) the inhibition of B7-1 binding to the CD28 (a soluble form of B7-1 may be used) in the presence of the candidate modulator is measured,
- (ii) inhibition of the binding of an antibody (that binds to the ligand binding face of CD28) to the CD28 in the presence of the candidate modulator is measured,
  - (b) a scintillation proximity assay (SPA) in which (i) or (ii) above are measured,
  - (c) an ELISA assay in which (i) or (ii) above are measured.

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The activity assay may test the effect of the candidate modulator on the ability of B7-1 or B7-2 to activate CD28. In such an assay, B7-1 or B7-2 may be present on a natural or artificial antigen-presenting cell and CD28 may be present on a T cell. CD28 activity may be detected by measuring the extent of T cell activation, for example by determining the extent of T cell proliferation (e.g. thymidine incorporation) or gene expression in the T cell (e.g. with microarrays).

The candidate modulator may be tested using the assays described in Green NJ, Xiang J, Chen J, Chen L, Davies AM, Erbe D, Tam S, Tobin JF. (2003) Structure-activity studies of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones binding to the immune regulatory protein B7.1. Bioorg Med Chem. 11, 2991-3013 or Erbe DV, Wang S, Xing Y, Tobin JF. (2002) Small molecule ligands define a binding site on the immune regulatory protein B7.1. J Biol Chem. 277, 7363-8.

#### The antibody and chimeric protein of the invention

The term "antibody" as used herein is understood to also include fragments and derivatives of the antibody which retain binding ability, unless the context requires otherwise. Such fragments/derivatives include Fv, F(ab') and F(ab')<sub>2</sub> fragments, as well as single chain antibodies, camelid antibodies and similarly acting proteins.

The antibody of the invention may be of any species, such as a mammalian or bird antibody, preferably a rodent (such as mouse) or primate (such as human) antibody. The antibody may be a chimeric antibody, a CDR-grafted antibody or a humanised antibody. The antibody may be monoclonal or polyclonal. The antibody is preferably an IgG antibody.

The invention also provides two types of chimeric protein that bind to a receptor. One type of chimeric protein comprises the sequence of a fragment of a ligand of the receptor, or sequence that is homologous to such a fragment. The sequence is capable of binding to an extracellular region of the receptor, as discussed further below. The chimeric protein also comprises the Fc region of an antibody, such as that of any of the types of antibody discussed above. Where the chimeric protein is administered to an individual the Fc region may be of an antibody of the same species as the individual.

The second type of chimeric protein provided by the invention comprises two Fv regions of an antibody. The Fv regions may be the same or different. One of the Fv regions is capable of binding to the extracellular region of the receptor (the "first" receptor). The other Fv region may bind the extracellular region of a "second" apposing receptor, this being the same type of receptor as the first receptor (with the second Fv binding at a location which is the same or different from the first Fv region) or an entirely different cell surface receptor, for example in the case where the first and second receptors are each expressed on the surfaces of two cells capable of interacting/contacting each other. Such cells may be any of the types of cell mentioned herein, including T cells.

In one embodiment the second Fv region of the second type of chimeric protein binds to a protein expressed on the surface of T cells, such as the T cell receptor, CD2, CD4, CD5, CD8, CD52 or CS1. The second Fv region may bind proteins expressed on the surface of other cells, such as CD48, CD58, CD59, B7-1 or B7-2. The term "receptor" when used in the present context refers to a protein expressed on surface of a cell (which may or may not be one which is capable of signal transduction, for example).

The antibody and chimeric protein of the invention are able to cause superagonistic signalling of a cell surface receptor when they bind to the receptor,

typically according to the mechanism illustrated in Figure 1. Thus the antibody or chimeric protein is able to cause activation of the receptor (i.e. cause the receptor to transduce a signal to the cytoplasm of the cell) without the need for additional costimulus of the receptor or cell. As mentioned above, in one embodiment the second type of chimeric protein comprises Fv regions able to bind to different types of receptors. Such a chimeric protein is preferably able to induce superagonistic signalling by both of the receptors which it binds.

The antibody and both types of chimeric protein bind the extracellular portion of the receptor at a membrane proximal region of the receptor, typically to a region of the receptor which is within 75Å of the cell membrane, such as within 60Å, 50Å or 40Å of the cell membrane. However the second type of chimeric protein of the invention typically also binds the extracellular portion of the second apposing receptor (as defined above), within 75Å of the cell membrane, such as within 60Å, 50Å or 40Å of the cell membrane.

Generally the antibody or chimeric protein will be capable of binding the native form of the receptor (at the extracellular regions discussed above) when the receptor is present on the surface of the cell where it occurs naturally.

The antibody or chimeric protein cause superagonistic signalling by sterically hindering the access of phosphatases (which tend to be large proteins), such as CD45, to the receptor (i.e. hindering contact of the phosphatase and receptor). In the case of the antibody or first type of chimeric protein such steric hindrance may be caused by the antibody binding to the receptor at one end (through the Fab of the antibody of the invention or the ligand sequence of the first type of chimeric protein) and typically binding to a protein on the surface of another cell (e.g. due to the Fc region of the antibody or chimeric protein binding to an Fc receptor expressed on a second cell), thus bringing the cell membrane of the two cells into close proximity in the region of the receptor.

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For the second type of chimeric protein, one of the Fv fragments of the chimeric protein will bind to the receptor, and in the case where the other Fv fragment is specific for a second type of receptor expressed on another cell, the other Fv fragment will bind to the second receptor and thus bring the cell membranes of the two cells into close proximity in the region of the first receptor.

For the antibody and both types of chimeric protein, the close proximities of the cell membranes in the region of the first receptor will sterically hinder phosphatases from accessing the receptor, leading to signal transduction or "triggering" of the receptor. The antibody or chimeric protein are typically capable of bringing the cell membranes of two cells within 200Å of each other, such as within 180Å, 150Å or 120Å of each other.

The antibody or chimeric protein will preferably bind orthogonally to the main axis of the domain of the receptor which is bound, such as at more than 60 degrees from the main axis of the bound domain of the receptor, for example at more than 70, 80 or 90 degrees. The antibody or chimeric protein will preferably lie substantially parallel to the cell surface when bound to the receptor (to ensure the membranes are brought into close proximity).

The antibody or chimeric protein will bind to an extracellular region of the receptor, generally to amino acids of the receptor that are exposed at the surface of the protein. The amino acids in the receptor that are bound may be present in a loop region or a  $\beta$ -strand of the receptor. Preferred loops and strand sequences are shown for key examples in Table 1. The antibody or chimeric protein may bind to any of the epitopes or part thereof shown in Table 1 or an equivalent homologous sequence from the membrane proximal region of other receptors.

The antibody of the invention does not bind only to the C'-D loop of CD28, and thus in one embodiment will bind both the C'-D loop of CD28 and another region of CD28. The antibody may be one which does not bind any portion of the C'-D loop of CD28. The antibody may or may not bind to the C'-D loop (or the equivalent loop) of any other member of the CD28 family of proteins. The antibody of the invention may or may not bind to any or all of the sequences shown in Table 3.

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The first type of chimeric protein of the invention may or may not bind to only the C'-D loop of CD28. The first type of chimeric protein may be one which does not bind to any portion of the C'-D loop of CD28. The first type of chimeric protein may or may not bind to the C'-D loop (or the equivalent loop) of any other member of the CD28 family of proteins. The first type of chimeric protein may or may not bind to any or all of the sequences shown in Table 3.

The second type of chimeric protein of the invention may or may not bind to

only the C'-D loop of CD28. The second type of chimeric protein may be one which does not bind to any portion of the C'-D loop of CD28. The second type of chimeric protein may or may not bind to the C'-D loop (or the equivalent loop) of any other member of the CD28 family of proteins. The second type of protein may or may not bind to any or all of the sequences shown in Table 3.

#### Receptors bound by the antibody and chimeric protein

The receptors which are bound by the antibody or chimeric protein of the invention are expressed on the cell surface. The receptor is capable of being phosphorylated (typically at one or more tyrosine residues in the cytoplasmic region of the receptor), and phosphorylation of the receptor will typically lead to its activation. The receptor will comprise a cytoplasmic domain that is dependent on extrinsic protein kinases to be phosphorylated. Thus the receptor will not have an intrinsic enzymatic (kinase or phophatase) activity. The receptor will typically comprise tyrosine-containing, activating ITAM motifs (YxxL/Ix<sub>7-12</sub>YxxL/I), inhibitory ITIM motifs (I/V/L/SxYxxL/V) or "switch" (TxYxxV/I; activating and inhibitory) signalling motifs (where x is any amino acid). These motifs are phosphorylated by cytoplasmic tyrosine kinases, such as the Src kinases, in competition with antagonistic tyrosine phosphatases, such as CD45. The signalling character of the receptors is defined exclusively by the nature of these motifs (ITAM vs ITIM: activating vs inhibitory).

The receptor may be a member of any surface protein superfamily, but is typically a member of the immunoglobulin superfamily. The receptor may be a member of the CD28 superfamily. The receptor may be any of the specific receptors which are shown in Table 1 or 2 or may comprise a sequence which is homologous to the sequence of any of these specific receptors. The receptor may be CD28, CTLA-4, ICOS, PD-1 or BTLA or comprise a sequence which is homologous to the sequence of any of these specific receptors.

The receptor may be of any of the species that are mentioned herein, and thus may be a mammalian or avian, preferably rodent (such as mouse or rat) or primate (such as human) receptor.

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The receptor may be naturally present on a cell of the immune system such as a T cell, B cell, myeloid cell, mast cell, NK cell or a granulocyte.

#### Screening methods of the invention

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The invention provides a method of obtaining an agent which is capable of superagonising the above-mentioned receptor which binds to the antibody and chimeric protein of the invention. The method comprises determining whether a candidate agent has any of the properties discussed above possessed by the antibody or chimeric protein of the invention which allows them to induce superagonistic signalling by a receptor. Thus the method will generally comprise determining whether a candidate agent is able to bind to an extracellular membrane proximal region of the receptor, and may also determine whether a candidate agent is able to bind

- at a particular location from the cell membrane (such as within 75Å of the cell membrane),
  - to particular sequences (such as the sequences mentioned in Table 1), or
- in a manner (such as orthogonal to the main axis of the bound receptor domain) which is discussed above for binding of the antibody or chimeric protein of the invention.

Suitable extracellular membrane proximal regions of a receptor may be identified using a sequence database search algorithm (e.g. BLAST) to search for the solved structure most related to the receptor in the protein structural database (PDB). This structure would then be used to identify membrane proximal regions (preferably β-strands) in the receptor by sequence alignment. Whether or not a candidate agent binds to the identified sequences could be determined by taking the midpoint of the strand and the side chains of amino acids two- and three-residues below this midpoint could then be mutated. Mutant forms of the receptor mutated at each of these residues would then be expressed (e.g. on suitable target cells that can be transfected stably or transiently, such as 293T cells), and used to screen for candidate agents that bound the non-mutated receptor but failed to bind the mutant receptor, for example using fluorescence-activated cell sorting. It is envisaged that only every second strand in a conventional beta barrel protein would need to be mutated. In the case of

a receptor which is a member of the immunoglobulin superfamily, this corresponds to 8-10 mutant lines being generated, in total. Examples of this process are shown in Figure 2 for the immediate CD28 family members (ICOS and CTLA-4) and for the PD-1 protein, which is representative of receptors not related to CD28.

Agents that induce superagonistic signalling by a receptor may also be identified using a peptide which comprises sequence from the extracellular membrane proximal region of a receptor or homologous sequence thereto. Such a sequence is typically 5 to 20 amino acids long, such as 10 to 15 amino acids long. In one embodiment the agent is identified using peptide arrays. The mapping of discontinuous epitopes can be performed using overlapping peptides derived from the entire primary sequence of a protein. The whole protein sequence is generated in the form of short overlapping peptides (for example each shifted by 3 amino acids), e.g. prepared by standard spot synthesis (Automated Spot Synthesiser, Abimed, Langenfeld, Germany) on Whatman 50 filter paper (Whatman, Maidstone, England). The C-termini of the peptides may be attached to cellulose via a (β-Ala)<sub>2</sub> spacer and the N-termini acetylated. The arrays may be subsequently probed either directly on the peptide membrane or after transfer to another surface (e.g. nitrocellulose) using the monoclonal antibody and a chemiluminescence-based detection system (ECL Western Blotting Detection System, Amersham Pharmacia Biotech).

Suitable candidate agents that can be tested in the above screening methods include antibody agents (for example, monoclonal and polyclonal antibodies, single chain antibodies, chimeric antibodies and CDR-grafted antibodies). Furthermore, combinatorial libraries, defined chemical identities, peptide and peptide mimetics, oligonucleotides and natural agent libraries, such as display libraries (e.g. phage display libraries) may also be tested. The candidate agents may be chemical compounds, which are typically derived from synthesis around small molecules. Batches of the candidate agents may be used in an initial screen of, for example, ten substances per assay, and the agents of batches which show the required property tested individually.

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Obtaining a superagonistic antibody

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The invention provides methods for obtaining a superagonistic antibody. In one embodiment the method comprises screening antibodies for the ability to superagonise a receptor, wherein the antibodies have been obtained either by immunizing an animal with the receptor or a homologue or fragment of the receptor, or from a combinatorial antibody library. Preferably the animal is immunized with a protein which comprises the sequences shown in Table 1, or a fragment thereof, or a homologue of such a sequence or fragment.

Whether or not an antibody is a superagonistic antibody may be ascertained by determining whether or not the antibody can bind an extracellular membrane proximal region of a receptor, for example using any of the suitable methods described above in the section of screening for superagonistic agents.

Alternatively the antibody can be tested in an activity assay to see whether or not it causes activation of the receptor. Receptors that are activated by the antibody will either transduce an activating signal or an inhibitory signal to the cell cytoplasm. In the case of receptors which transduce an activating signal, as in the case of CD28, the activity which is tested may be activation of the cell. This can be determined using functional screens based on, for example, cell proliferation, increased cellular calcium, enhanced tyrosine phosphorylation of proteins in the cell or the production of/release of substances by the cell, e.g. IL-2 production. In the case of receptors that transduce inhibitory signals when activated, activation of such receptors can be ascertained by detection of any of the changes which occur to the receptor or the cell when such a signal is transduced, such as changes in the extent of phosphorylation of one or more proteins in the cell.

The binding or activity assay may be carried out in vitro (inside or outside a cell) or in vivo.

In one embodiment of the method the antibody is obtained by immunising an animal with a peptide comprising a sequence of length 5 to 20 amino acids which represents an extracellular membrane proximal region of the receptor, or a homologue of such sequence, and obtaining the antibody produced by the animal against said sequence. Alternatively the antibody may be obtained by selecting an antibody from a combinatorial library based on its ability to bind a peptide

comprising a sequence of length 5 to 20 amino acids which represents an extracellular membrane proximal region of the receptor, or a homologue of such sequence.

In one embodiment the peptide which is used to immunise the animal or select an antibody from a library only comprises sequence from the receptor, or a homologue thereof, and does not comprise any additional sequence. In this embodiment the peptide will only be 5 to 20 amino acids long. However in other emobodiments the peptide comprises other sequence to the N-terminus and/or C-terminus of the receptor sequence, such as sequence which is different from (and typically not homologous to) receptor sequence.

#### Antibodies

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Various types of antibodies are mentioned herein, including antibodies obtained by immunisation. Such antibodies may be raised against specific epitopes/sequences. An antibody, or other compound, "specifically binds" to a sequence when it binds with preferential or high affinity to the sequence for which it is specific but does not bind or binds with only low affinity to other sequences. A variety of protocols for competitive binding or immunoradiometric assays to determine the specific binding capability of an antibody are well known in the art (see for example Maddox *et al*, J. Exp. Med. 158, 1211-1226, 1993). Such immunoassays typically involve the formation of complexes between the specific sequence and its antibody and the measurement of complex formation.

Means for preparing and characterising antibodies are well known in the art, see for example Harlow and Lane (1988) "Antibodies: A Laboratory Manual", Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY. For example, an antibody may be produced by raising antibody in a host animal.

A method for producing a polyclonal antibody comprises immunising a suitable host animal, for example an experimental animal, with the immunogen and isolating immunoglobulins from the animal's serum. The animal may therefore be inoculated with the immunogen, blood subsequently removed from the animal and the IgG fraction purified.

A method for producing a monoclonal antibody comprises immortalising cells which produce the desired antibody. Hybridoma cells may be produced by fusing spleen cells from an inoculated experimental animal with tumour cells (Kohler and Milstein (1975) *Nature* 256, 495-497).

An immortalized cell producing the desired antibody may be selected by a conventional procedure. The hybridomas may be grown in culture or injected intraperitoneally for formation of ascites fluid or into the blood stream of an allogenic host or immunocompromised host. Human antibody may be prepared by in vitro immunisation of human lymphocytes, followed by transformation of the lymphocytes with Epstein-Barr virus.

For the production of both monoclonal and polyclonal antibodies, the experimental animal is suitably a goat, rabbit, rat, mouse, guinea pig, chicken, sheep or horse. If desired, the immunogen may be administered as a conjugate in which the immunogen is coupled, for example via a side chain of one of the amino acid residues, to a suitable carrier. The carrier molecule is typically a physiologically acceptable carrier. The antibody obtained may be isolated and, if desired, purified

#### The peptide of the invention

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The invention also provides a peptide of length 5 to 20 amino acids comprising a sequence which binds to the superagonistic antibody of the invention. The peptide may have a length of 10 to 15 amino acids. The peptide may comprise sequence from an extracellular membrane proximal region of any of the receptors mentioned herein or have a homologous sequence thereto (such sequence may have a length of 5 to 20 amino acids). The peptide may thus comprise any of the sequences shown in Table 1 or homologues of such sequences.

#### Therapeutic aspects of the invention

The invention provides substances which can be used to treat a patient. The patient is typically a human or animal, such as a mammal or bird, for example a cow, sheep, goat, pig, camel, horse, dog, cat, goose, duck or chicken.

The modulator of CD28 which is identified from a structural model or structural coordinates of CD28 can be used to modulate the immune system of a

patient. Such modulators will either agonise or antagonize CD28 (i.e. cause or contribute to an increase or decrease, respectively, in CD28 signalling activity). Modulators which agonise CD28 may be used to stimulate the activity of T cells (which express CD28) and thus to stimulate an immune response against an antigen. Such modulators may therefore be used in the prevention or treatment of a disease caused by a pathogenic agent, such as a virus, microorganism (for example a bacterium) or multicellular organism; or in the prevention or treatment of a cancer.

Modulators which antagonise CD28 may be used to inhibit the activity of T cells, and thus to inhibit an immune response to an antigen. Such modulators may be used to prevent or treat an autoimmune disease (such as rheumatoid arthritis or asthma), allergy or transplantation rejection.

The superagonistic antibodies, chimeric proteins and agent described herein may also be used in the therapy of patients to prevent or treat a disease. These substances may be used to modulate the state of a cell on which the relevant receptor is present. Thus the substance may activate or inhibit cell activity depending on whether the activated receptor transduces a stimulatory or inhibitory signal to the cytoplasm of the cell. The modulation of the cell may thus be used to treat a disease caused by the cell or a disease which can be alleviated or prevented by the cell.

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In a preferred embodiment the cell is a cell of the immune system (e.g. any such cell mentioned herein) and therefore superagonistic antibodies, chimeric proteins and agents may be used to modulate the immune response of a patient. Superagonistic antibodies, chimeric proteins and agents which stimulate an immune response may be used in the prevention or treatment of a disease caused by a pathogenic agent, such as a virus, microorganism (for example a bacterium) or multicellular organism; or in the prevention or treatment of a cancer. Superagonistic antibodies, chimeric proteins and agents which inhibit an immune response may be used to prevent or treat an autoimmune disease (such as rheumatoid arthritis or asthma), allergy or transplantation rejection.

The patient may also be treated by generating a superagonistic antibody response in the patient by immunisation with a peptide that stimulates the generation of such a response. The antibody that is generated will be specific to a sequence present in the peptide. The peptide will comprise sequence from the extracellular

membrane proximal region of a receptor, or sequence which is homologous thereto.

Such receptor sequence may be any of the membrane proximal sequences of a receptor (or homologues thereof) mentioned herein. Thus the peptide may be any of the peptides mentioned herein which comprise such sequence.

In one embodiment a nucleic acid capable of expressing any of the abovementioned therapeutic substances is administered to the patient. Such a nucleic acid typically comprises a region which encodes the therapeutic substance and a control region which causes expression of the coding sequence, such as a promoter. Thus the nucleic acid may be in the form of a vector.

The substances mentioned herein

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The modulators, antibodies, chimeric proteins, peptides and nucleic acids mentioned herein may be present in a substantially isolated form. They may be mixed with carriers or diluents which will not interfere with their intended use and still be regarded as substantially isolated. They may also be in a substantially purified form, in which case they will generally comprise at least 90%, e.g. at least 95%, 98% or 99%, of the proteins nucleic acids or dry mass of the preparation.

#### Homologues

Homologues of protein sequences are referred to herein. Such homologues typically have at least 50% homology, preferably at least 60%, 70%, 80, 90%, 95%, 97% or 99% homology, for example over a region of at least 15, 20, 30, 100 more contiguous amino acids. The homology may be calculated on the basis of amino acid identity (sometimes referred to as "hard homology").

For example the UWGCG Package provides the BESTFIT program which can be used to calculate homology (for example used on its default settings) (Devereux et al (1984) Nucleic Acids Research 12, p387-395). The PILEUP and BLAST algorithms can be used to calculate homology or line up sequences (such as identifying equivalent or corresponding sequences (typically on their default settings), for example as described in Altschul S. F. (1993) J Mol Evol 36:290-300; Altschul, S, F et al (1990) J Mol Biol 215:403-10.

Software for performing BLAST analyses is publicly available through the National Center for Biotechnology Information (http://www.ncbi.nlm.nih.gov/). This algorithm involves first identifying high scoring sequence pair (HSPs) by identifying short words of length W in the query sequence that either match or satisfy some positive-valued threshold score T when aligned with a word of the same length in a database sequence. T is referred to as the neighbourhood word score threshold (Altschul et al, supra). These initial neighbourhood word hits act as seeds for initiating searches to find HSPs containing them. The word hits are extended in both directions along each sequence for as far as the cumulative alignment score can be increased. Extensions for the word hits in each direction are halted when: the cumulative alignment score falls off by the quantity X from its maximum achieved value; the cumulative score goes to zero or below, due to the accumulation of one or more negative-scoring residue alignments; or the end of either sequence is reached. The BLAST algorithm parameters W, T and X determine the sensitivity and speed of the alignment. The BLAST program uses as defaults a word length (W) of 11, the BLOSUM62 scoring matrix (see Henikoff and Henikoff (1992) Proc. Natl. Acad. Sci. USA 89: 10915-10919) alignments (B) of 50, expectation (E) of 10, M=5, N=4, and a comparison of both strands.

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The BLAST algorithm performs a statistical analysis of the similarity between two sequences; see e.g., Karlin and Altschul (1993) *Proc. Natl. Acad. Sci.* USA 90: 5873-5787. One measure of similarity provided by the BLAST algorithm is the smallest sum probability (P(N)), which provides an indication of the probability by which a match between two amino acid sequences would occur by chance. For example, a sequence is considered similar to another sequence if the smallest sum probability in comparison of the first sequence to the second sequence is less than about 1, preferably less than about 0.1, more preferably less than about 0.01, and most preferably less than about 0.001.

The homologous sequence typically differs by at least 1, 2, 5, 10, 20 or more mutations (each of which may be a substitution, deletion or insertion of an amino acid). These mutations may be measured across any of the regions mentioned above in relation to calculating homology. The substitutions are preferably conservative substitutions. These are defined according to the following Table. Amino acids in

the same block in the second column and preferably in the same line in the third column may be substituted for each other:

ALIPHATIC	Non-polar	GAP
		ILV
	Polar – uncharged	CSTM
·		NQ
	Polar - charged	DE
		KR
AROMATIC		HFWY

#### 5 Administration

The formulation of any of the therapeutic substances mentioned herein will depend upon factors such as the nature of the substance and the condition to be treated. Any such substance may be administered in a variety of dosage forms. It may be administered orally (e.g. as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules), parenterally, subcutaneously, intravenously, intravenously, intrasternally, transdermally or by infusion techniques. The substance may also be administered as suppositories. A physician will be able to determine the required route of administration for each particular patient.

Typically the substance is formulated for use with a pharmaceutically acceptable carrier or diluent. The pharmaceutical carrier or diluent may be, for example, an isotonic solution. For example, solid oral forms may contain, together with the active compound, diluents, e.g. lactose, dextrose, saccharose, cellulose, corn starch or potato starch; lubricants, e.g. silica, talc, stearic acid, magnesium or calcium stearate, and/or polyethylene glycols; binding agents; e.g. starches, arabic gums, gelatin, methylcellulose, carboxymethylcellulose or polyvinyl pyrrolidone; disaggregating agents, e.g. starch, alginic acid, alginates or sodium starch glycolate; effervescing mixtures; dyestuffs; sweeteners; wetting agents, such as lecithin, polysorbates, laurylsulphates; and, in general, non-toxic and pharmacologically

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inactive substances used in pharmaceutical formulations. Such pharmaceutical preparations may be manufactured in a known manner, for example, by means of mixing, granulating, tabletting, sugar-coating, or film coating processes.

Liquid dispersions for oral administration may be syrups, emulsions and suspensions. The syrups may contain as carriers, for example, saccharose or saccharose with glycerine and/or mannitol and/or sorbitol.

Suspensions and emulsions may contain as carrier, for example a natural gum, agar, sodium alginate, pectin, methylcellulose, carboxymethylcellulose, or polyvinyl alcohol. The suspensions or solutions for intramuscular injections may contain, together with the active compound, a pharmaceutically acceptable carrier, e.g. sterile water, olive oil, ethyl oleate, glycols, e.g. propylene glycol, and if desired, a suitable amount of lidocaine hydrochloride.

Solutions for intravenous or infusions may contain as carrier, for example, sterile water or preferably they may be in the form of sterile, aqueous, isotonic saline solutions.

A therapeutically effective amount of substance is administered. The dose may be determined according to various parameters, especially according to the substance used; the age, weight and condition of the patient to be treated; the route of administration; and the required regimen. Again, a physician will be able to determine the required route of administration and dosage for any particular patient. A typical daily dose is from about 0.1 to 50 mg per kg, preferably from about 1.0 mg per kg to 10 mg per kg of body weight, according to the activity of the specific therapeutic substance, the age, weight and condition of the subject to be treated, the type and severity of the disease and the frequency and route of administration. Preferably, daily dosage levels are from 5 mg to 2 g.

The following Examples illustrate the invention:

#### Examples

#### Overview of crystallisation strategy

In order to undertake crystallization trials with glycoproteins, such as the CD28 homodimer, it is generally necessary to produce large amounts of protein (>10 milligrams). For this the glutamine synthetase-based Chinese hamster ovary cell expression system (Lonza Biologics Plc, UK) was chosen, which is one of the few

eukaryotic expression systems capable of glycoprotein production at this level. The Lec3.2.8.1 cell line was used as the expression host as this provides the option of enzymatically removing unnecessary glycosylation after protein folding and secretion has taken place, which generally favours crystallization. In order to enhance homodimerization, the protein was expressed in the form of a fusion protein with the Fc region of immunoglobulin, which is itself a homodimer. Because the link between the CD28 portion and the Fc is extremely flexible (which will generally discourage crystallization), the construct was prepared in a way that made it thrombin-cleavable.

It was found that producing active, thrombin-cleavable protein depended on the location of the cleavage site. When the cleavage site was too close to the ligand binding domain (to make a more compact protein for crystallization), the protein produced was mis-folded.

In general removal of the N-linked glycans from a glycoprotein substantially enhances its ability to crystallise. Unexpectedly, and in marked contrast to other cell surface glycoproteins, which are generally very stable and active after deglycosylation, the CD28 homodimer proved to be very unstable after deglycosylation with the enzyme endoglycosidase H at the slightly acidic pH at which this enzyme is active. Therefore it was necessary to leave the glycosylation of CD28 intact. The glycosylated form of the homodimer failed to crystallise in more than 100 trials.

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To reduce the impact of the glycosylation, therefore, an alternative strategy was employed, in which Fab fragments of anti-CD28 antibodies were prepared and crystallised with CD28. Fab fragments are almost invariably unglycosylated, so the formation of complexes with the Fab can be expected to reduce the impact of the glycans by 80%, regardless of where they bind the protein of interest (a Fab is four times the size of the CD28 monomer). The likelihood that the complex of the Fab and protein of interest will crystallise depends on the overall shape of the complex, (i.e. its "compactness") and on the chemical properties of the surfaces of the complex involved in forming crystal lattice contacts. Because the surface of the complex that will form lattice contacts cannot be predicted a priori, it is impossible to predict whether a given Fab will give crystals when complexed with the protein. Not unexpectedly, therefore, the homodimer still failed to crystallize after being complexed with one Fab molecule

per homodimer for two different antibodies (5.11A1 and 9D7), or two Fabs per homodimer for one of these antibodies (5.11A1), in >100 trials per complex.

In addition the stalk region was expected to create problems. The key to obtaining crystals was to prepare monomeric CD28 by gentle reduction and alkylation of the interchain disulphide bond in the stalk-like region of the homodimer. The expectation was that the presence of an intact disulphide in the stalk might rigidify the stalk, making the overall structure less compact. Two complexes formed with the monomer and two different Fabs (5.11A1 and 9D7) gave crystals, but only one of these crystal forms (obtained with 5.11A1 Fab fragments) proved to be suitable for data collection. Other antibodies may also have been useful in crystallising CD28, including antibodies that bind to the same loop of CD28 as bound by 5.11A1 (the C'-D loop) or that bind to the ligand binding site of CD28. Suitable antibodies are described in US-A1-2003/0166860 and Luhder et al (2003) J. Exp. Med., 197, 955-66.

#### Preparation of CD28 homodimer

#### (i) Construct generation

The polymerase chain reaction (PCR) was used to amplify complementary DNA (cDNA) encoding the signal peptide sequence of mouse immunoglobulin heavy chain and the extracellular domain of CD28 (residues 1-134 of the mature polypeptide; SEQ 20 ID NO:1) from 44 ng of the plasmid, pKGe1145. The oligonucleotides used in the reaction added, at the 5' end, an Xba I cleavage site and 24 nt of the rat CD4 5' untranslated region and, at the 3' end, codons for the thrombin cleavage site, LVPRGS. The sequences of the oligonucleotide primers used for this were (oligonucleotide sequences are given in 5' to 3' direction) CD28T\_5': TAG TAG TCT AGA CCC CAT CCG CTC AAG CAG GCC ACC ATG GAT TGG CTG CGG AAC TTG; and CD28T\_3': CTA CCA CTA CCC CTG GGT ACC AGG GGC TTA G. In a second reaction, cDNA encoding the heavy chain constant (C) region-2 and C region-3 domains of murine Ig (residues 103-323 of the secreted protein) was amplified by PCR from 44 ng of pKGe1145. At the 3' end, the oligonucleotides added an Xba I restriction site to aid cloning. The NH2-terminus of the protein encoded by the Ig cDNA had the sequence GSKPSIS rather than GCKPCIC. The sequences of the oligonucleotide primers for this reaction were Ig\_5': CTA AGC CCC TGG TAC CCA GGG GTA GTG GTA G; and Ig\_3': CTA CTA TCT AGA TTA TTT ACC AGG AGA GTG GGA G. The PCR conditions for both reactions were: denaturation at 94°C for 15s, annealing at 59°C for 30s, extension at 68°C for 210s; 2.5U of Accuzyme polymerase (Bioline Ltd, U.K.), 300 nM oligonucleotides and 200  $\mu$ M dNTPs were used and the reactions run for 20 cycles.

In a third reaction, PCR was used to anneal the two initial products together to generate cDNA encoding a chimera consisting of the CD28 extracellular domain fused to murine IgGFc via a thrombin cleavable sequence (called the CD28TFc chimera; SEQ ID NO:2). Ten microlitres of each of the initial PCR reaction product mixtures was used as template and 300 nM of the CD28\_5' and Ig\_3' oligonucleotides was also added to the mix. The PCR conditions were otherwise identical to the first set except that they were run for only 4 cycles. The PCR product was gel-purified, cut with Xba I and cloned into the Xba I site of pEE14 for expression in the glutamine synthetase-based gene expression system (Lonza Biologics Plc, UK). The plasmid construct was then sequenced using dideoxy sequencing.

#### (ii) Expression of the CD28TFc chimera

Lec3.2.8.1 cells, 2 x 10<sup>6</sup>/flask, were transfected with 20 μg of DNA/flask for 3h using Pfx-8 lipids (Invitrogen Inc), and then the cells were cloned the following day by plating out at 2 x 10<sup>6</sup> cells/96-well plate. After 2 weeks, the clones expressing the highest amounts of CD28TFc were selected by Western-blotting using the semi-quantitive ECL detection system (Amersham-Pharmacia, UK) and an anti-mouse Fc primary antibody (Sigma-Aldrich Co.). The best-expressing clone was expanded and grown to confluence in bulk culture in Cell Factories (Nunc A/S, Denmark) containing immunoglobulin-free medium (Invitrogen-Gibco Ltd, UK) in the presence of 2mM sodium butyrate. The supernatant was harvested after approximately four weeks and clarified by centrifugation at 5,000g.

#### (iii) CD28TFc purification

The spent, clarified medium was concentrated to approximately 1/6 of the original volume using a Masterflex L/S concentrator (Helixx Technologies, Inc.). The sample was then buffer-exchanged against the original volume of 3M NaCl, 1.5M

glycine, pH 8.5 high-salt buffer and the protein incubated with Protein A Sepharose beads (Sigma-Aldrich Co.) using 10 mls of swollen beads/litre of concentrated supernatant at 1 litre of supernatant/5 litre conical flask or beaker. The pH was adjusted to pH 8.5 with 2.75 M Tris, pH 8.5 to allow binding of the CD28TFc to Protein A overnight with gentle stirring at 4°C.

The beads were allowed to settle for 2 h prior to siphoning off the depleted supernatant. The settled beads were then transferred to 50 ml Falcon tubes (Becton Dickinson Biosciences, UK) and recovered by centrifugation at 200g. The beads were transferred to a 30 ml column (Biorad, UK) and then washed with 300 mls of cold phosphate-buffered saline, 0.5 M NaCl, pH 8.3. The column was eluted with 0.1 M citric acid, pH 3.0 into 10 x 2 ml fractions in glass tubes containing 0.4 ml of 2.75M Tris, pH 8.5 for immediate neutralization of the citric acid. Fractions containing CD28TFc according to analysis by 12% sodium dodecyl sulphate polyacrylamide gel electrophoresis (SDS-PAGE) were concentrated to 0.5ml or no higher concentration than 20 mg/ml using a Centriprep 10 concentrator (Millipore Corp). The protein was then applied to a Superdex 200 H/R gel filtration column (Amersham Biosciences) preequilibrated with 10 mM Hepes, 140 mM NaCl, pH 7.4 (HBS buffer) for up to three successive runs. Eluting fractions were monitored for absorbance at 280 nm. Proteincontaining fractions were examined by SDS-PAGE. Each cycle of batch purification yielded ~9 mgs of CD28TFc; up to 7 batch-purfications was required to deplete all the CD28TFc per set of 6 cell factories (~5 litres of starting tissue culture supernatant).

#### (iv) Thrombin protease cleavage of CD28TFc

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The most-pure fractions containing CD28TFc were pooled for thrombin cleavage. Initial trial titrations dictated the use of the following conditions for large-scale cleavage of CD2TFc: lyophilized thrombin (Sigma-Aldrich Co.) was re-hydrated in HBS buffer to a concentration of 1U/µl and this was then added to the CD28TFc at 0.11 µl/6 µg of protein for overnight digestion at 37°C. The reaction was stopped by addition of freshly re-hydrated benzamidine to a final concentration of 1mM. A 12% non-reducing SDS-PAGE gel was used to confirm the extent of cleavage.

#### (v) Purification of the CD28 homodimer

The pH of the thrombin-cleaved protein was adjusted to pH 8.5 using 2.75M Tris pH 8.5, prior to concentration to 0.5 ml using a Centriprep 10 concentrator (Millipore Corp). Fresh Protein A beads were washed and rehydrated to a final volume of ~5 mls, prior to being packed into a 0.7 cm x 20 cm Econo-column (Bio-Rad, U.K.) and then equilibriated with HBS, pH 8.5 at 4°C. The concentrated protein was then applied to the column, allowed to run into the bed, and then sequential fractions were eluted by addition of 0.5 ml of HBS, pH 8.5 to the top of the bed every 10 minutes for 2h. The absorbance of each fraction was determined at 280 nm. The extent of separation of the Fc from the thrombin-released CD28 homodimer was determined by 12% SDS-PAGE analysis of the fractions under non-reducing conditions. The critical steps for good separation were (1) to allow the protein to pass slowly through the column and (2) to conduct the separation at 4°C. The homodimer was concentrated to 0.5 ml and subjected to gel-filtration on a Superdex 75 H/R column (Amersham Biosciences). The purified homodimer was used for crystallization trials, reduced and alkylated for other crystallization trials (see below), or frozen at -80°C for future use.

#### Preparation of Fab fragments of 5,11A1 antibody

Fab fragments were prepared using the Pierce Biotechnology ImmunoPure® Fab Preparation Kit, as briefly outlined below.

#### (i) Fab fragment generation and purification

Nine millilitres of whole, purified 5.11A1 antibody at 0.3 mg/ml in PBS was concentrated to 1 ml and then diluted to 10 mls with 20 mM sodium phosphate, 10 mM EDTA, pH 7 and then re-concentrated to 0.5 ml. To this was added 0.5 ml of 20 mM sodium phosphate, pH 7 containing 3.5 mg/ml cysteine•HCl. The 1 ml mixture was then added to 0.5 ml of a 50% slurry of Sepharose-immobilized Papain supplied with the kit, which had been pre-equilibrated with 20 mM sodium phosphate pH 7 containing 3.5 mg/ml cysteine•HCl. This was then incubated for 5 hours in a shaking water bath at 37°C. The cleaved Fab and Fc fragments and undigested IgG were separated from the Immobilized Papain beads by centrifugation at 1000g and the beads rinsed with 1.5 ml of the ImmunoPure IgG Binding Buffer supplied with the kit. The wash was then combined with the crude digest and the mix applied to a Sepharose-immobilized Protein

A column pre-equilibrated with 13 ml of ImmunoPure IgG Binding Buffer. The column was washed with 6.0 ml of the Binding Buffer and the eluate containing the Fab fragments collected (9 mls in total). The eluate was concentrated to 0.5 ml and applied to a Superdex 200 H/R gel filtration column (Amersham Biosciences) pre-equilibrated with HBS buffer. Eluting fractions were monitored for absorbance at 280 nm. Protein-containing fractions were examined by SDS-PAGE.

#### Preparation of a crystallizable form of CD28

#### (i) Reduction and alkylation of CD28

CD28 has an interchain disulphide bond within the "stalk-like" region that is largely responsible for homodimerization. It was speculated that its location within the stalk would render it more sensitive to reducing agents than the "canonical" disulphide bond and one other disulphide buried within the ligand-binding domain. If true this meant that monomeric CD28 could be generated which was native-like and fully active for ligand and antibody binding. The minimum concentration of reducing agent required to release the monomer was ascertained by titrating the reducing agent, dithiothreitol (DTT). The reduced cysteines in the protein and excess DTT were each then inactivated by alkylation with a 2.2-fold molar excess of iodoacetamide (IAA). This titration indicated that the optimal conditions were 12.5 µM protein, 1.5mM DTT and 3.3 mM IAA. The reduced protein sample, generally ~4 ml, was finally concentrated to 0.5 ml and separated from unreduced homodimer by gel-filtration on a Superdex 75 H/R column (Amersham Biosciences).

#### Crystallographic methods

#### 25 (i) Crystallization and data collection

The CD28/5.11A1 Fab complex was formed by incubating a 2:1 molar ratio of CD28 and Fab, followed by concentration of the protein mixture to 15.6 mg/ml in HBS. (the extinction coefficient,  $\epsilon$ , of CD28 is 1.7 and that of the Fab is 1.4). Crystals were grown at 18°C in 0.2  $\mu$ l hanging drops (0.1  $\mu$ l of the protein mixture plus 0.1  $\mu$ l of precipitating reagent) set up using a Cartesian Robot (APS Robotics & Integration, Ilc; Brown et al (2003) J. Appl. Cryst. 36, 315-18). The precipitating reagent consisted of a mixture of 0.2 M magnesium formate and 20% polyethylene glycol 3350 in water.

Crystals appeared in 5-7 days and were cooled to 100K in the precipitating reagent with glycerol added to a final concentration of 10%, using a Cryojet liquid nitrogen system for data collection (Oxford Instruments, Abingdon, UK). Crystals belong to space group C2 with unit cell dimensions a = 191.2, b = 47.4, c = 71.8 Å and a calculated solvent content of 56-58% for one CD28 monomer and one Fab molecule per asymmetric unit (ignoring the effects of glycosylation). The 2.7Å resolution data were collected from a single crystal at 100K at Beamline ID2 at the European Synchrotron Radiation Facility using a FReLoN CCD. One hundred and fifty-eight 1° rotation images were collected and reduced with HKL2000 (Otwinowski and Minor (1997) Methods Enzym. 276, 307-26).

#### (ii) Structure determination and refinement

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The structure was solved by molecular replacement in XPLOR v3.851 (Brunger (1992) X-PLOR Version 3.1. A system for X-ray crystallography and NMR. Yale University Press, New Haven, CT.) using a set of search models generated from a single Fab structure (PDB accession no. 15c8) by varying the elbow angle in 2° steps using an XPLOR script. A single unambiguous solution was found when the elbow angle was altered by -8° as defined by the script. After rigid body refinement of each domain of the Fab in CNS (Brunger et al. (1998) Acta Cryst. D54, 905-21), the R-factor was 44.4%. Initial electron density maps phased with Fab alone showed very limited, if any, electron density for the CD28 molecule. The Fab model was mutated to the sequence of 5.11A1 before proceeding with two cycles of manual rebuilding in O (Jones et al (1990) O: A macromolecular modelling environment. Crystallographic and modeling methods in molecular design. Bugg and Ealick, Eds. Springer-Verlag Press 189-95) and positional refinement in CNS, reducing the R-factor to 36.4%. A molecular replacement solution for CD28 was then found by using only regions of human CTLA-4 (from PDB 1i8l) with strong sequence homology to CD28, i.e. all the  $\beta$ -strands (except C') and the EF and FG loops, as a search model and by fixing the refined Fab structure. In order to avoid model bias, the refined constant regions of the Fab were replaced with the unaltered constant domains from PDB 15c8 by superposition using SHP (Stuart et al (1979) J. Mol. Biol. 134, 109-42), and the positions were fixed during refinement. The variable regions of the Fab and the CD28 monomer were refined in X-PLOR v3.851

using positional refinement followed by grouped and restrained individual B factor refinement along with manual rebuilding in O. All refinement procedures used data from 25.0-2.7Å and excluded 5% of reflections randomly selected for generation of the R<sub>free</sub> data set. The anisotropy of the data was corrected for using X-PLOR and the data were sharpened for all but the last round of refinement. The current model has an R factor of 25.3% and an R<sub>free</sub> of 33.4% against all data to 2.7Å. The model includes the CD28 monomer (excluding its C-terminal stalk) from residues 2 to 118, excluding residues Leu28 and Phe29, which are poorly ordered, and the Fab, but with none of the sugar chains built onto the CD28. The model has 76% of residues in the most favoured regions of the Ramachandran plot, with a further 21% in additionally allowed regions.

#### The structure of a CD28-superagonist antibody complex

The ligand-binding V-set IgSF domain of the CD28 monomer, solved in complex with 5.11A1 Fab, is very similar to the equivalent region of CTLA-4. Lattice contacts generate a plausible CD28 homodimer. Whilst this dimer is similar to the CTLA-4 homodimer (which is bivalent), the arrangement of the monomers in CD28 is sufficiently distinct to suggest an explanation for the apparent monovalence of CD28, i.e. the membrane proximal domains of ligands competing for each ligand binding site are likely to clash. Cryoelectron microscopic analyses show that both classes of antibodies are bivalent, ruling out aggregation-based explanations for the differential signalling effects of conventional versus superagonistic antibodies. The 5.11A1 Fab fragment binds orthogonally to the surface formed by the CC'C" strands of CD28, favouring the C'C" "edge" of the monomer. This places the two long axes of the Fabs parallel to each other and the cell surface. In contrast, the epitopes of the conventional antibodies are close to the ligand binding "top" of the homodimer.

#### Signalling by receptors dependent on extrinsic kinases

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The existence of two classes of activating anti-CD28 antibodies, i.e. costimulatory antibodies and superagonists, greatly simplifies the analysis of signalling by this archetypal costimulatory receptor. The observation that the two antibody classes have homologous effects in two different species, and that these effects are predictable simply according to the location of their epitopes, rules out

trivial explanations for the distinct signalling properties of these antibodies, e.g. affinity differences. Instead, the receptor-triggering problem is reduced to a comparison of the structural properties of the complexes that these two types of antibodies form with CD28.

From the present crystal structure of the complex of CD28 with a superagonistic antibody, it can be deduced that an antibody-induced increase in the net phosphorylation of the cytoplasmic domain of a given cell surface receptor, due to changes in the rates of phosphorylation and dephosphorylation of it, results in the triggering of that receptor (see Figure 1). In more detail, the antibodies hold the cell surface at certain distances from an immobilizing substrate (i.e. other, Fc receptorbearing cells, in vivo or plastic, in vitro), such that the membrane separation in the region of the immobilized antibody and receptor will differentially exclude, from the immediate vicinity of the receptor, other molecules whose extracellular domains are comparable in size or larger than CD28-antibody complexes, such as the tyrosine phosphatase, CD45. In contrast, tyrosine kinases, e.g. p56lck, will be unaffected because they are small and/or attached to the inner leaflet of the membrane. The result is that, overall, the phosphorylation of CD28 will be favoured over its dephoshorylation (by CD45), with the net increase in phosphorylation amounting to receptor triggering. Superagonists are more potent than conventional antibodies because they bind epitopes close to the membrane rather than at the "top" of the molecule, leading to more efficient segregation of, e.g. CD45, and therefore a larger increase in the net phosphorylation of CD28.

The important corollary of this explanation is that antibodies that bind the membrane-proximal epitopes of the large number of other cell surface molecules not belonging to the CD28 subset of the immunoglobulin superfamily, but sharing the key signalling property of CD28-subset molecules, *i.e.* a reliance on extrinsic tyrosine kinases, for example PD-1 and BTLA, should also potently invoke the activating or inhibitory signalling properties of those molecules in precisely the same way, allowing the manipulation of cell behaviour with such antibodies.

#### PD-1 and BTLA

Programmed Death (PD)-1 protein modulates the responses of previously activated T- and B-cells in secondary lymphoid organs or peripheral (parenchymal) tissues. PD-1 is expressed on a subset of thymocytes and upregulated on activated T, B and myeloid cells. The PD-1 ligands, B7-H1 and B7-DC, are more widely expressed than those of CD28 family members and are induced by pro-inflammatory agents on monocytes and dendritic cells and on activated but not resting B cells. B7-DC is expressed in a variety of peripheral tissues, including heart, pancreas, lung and liver. The B and T lymphocyte attenuator (BTLA), is also expressed on activated T and B cells, but attenuates production of IL-2 after binding a different peripherally expressed B7-related protein, called B7x.

PD-1 and BTLA are structurally comparable to other members of the CD28 family only insofar as the proteins also consist of a single V-set IgSF domain supported on stalks, and the cytoplasmic domains contain immunoreceptor tyrosine-based motifs (inhibitory in these two cases). The sequences of the IgSF domains of PD-1 and BTLA indicate that these proteins are unrelated and *do not* belong to the same subset of the IgSF as CD28. Consistent with the view that PD-1 is involved in maintaining tolerance in normal T cells in the periphery, mice lacking the gene develop a variety of autoimmune-like diseases dependent on the genetic background, including lupus-like arthritis and glomerulonephritis, and have increased serum IgG3 and augmented B-cell proliferative responses to anti-IgM *in vivo*.

Activating signalling by PD-1 and BTLA, because these molecules are inhibitory, would be expected to dampen a variety of peripheral immune pathologies. Signalling of this type could be stimulated by the binding of superagonistic antibodies to the membrane proximal regions of these proteins. A set of additional molecules, each of which has inhibitory immunoreceptor tyrosine-based signalling motifs and are therefore targets for generating superagonists, is shown in Table 2.

#### Identifying epitopes for superagonists

The procedure is as follows. The "lower", membrane-proximal half of the membrane proximal domain of a given structure, e.g. CD28 in Figure 2A, is identified by visual inspection of the structure. Superagonistic agents bind residues in

this region. For identifying superagonistic agents in receptors closely related to the known structure, the equivalent regions are identified in an alignment of the sequence of the known structure with that of the related proteins as shown in Figure 2A. To identify the epitopes of superagonistic antibodies in other molecules that have the requisite signalling properties but for which there is no structure, e.g. PD-1 in Figure 2B, a structural model is identified by alignment of the sequence with that of the most similar molecule of known structure in the Protein Data Bank (in the example in Figure 2B, the variable domain of the Ig kappa chain is the structure with the most similar sequence to PD-1). The "lower", membrane proximal half of this domain is highlighted on the structure by visual inspection and the equivalent regions are identified in the sequence alignment. To screen for superagonists, the second and third residues "down" (i.e. toward the membrane) in the marked epitopes shown in parts A and B are identified as shown in Figures 2C and 2D. These residues, singly or together preferably form at least part of the epitopes of antibodies or other superagonistic agents, as binding to these residues will require that the binding of the agent is parallel with the cell membrane. These residues can therefore be mutated in proteins used for screening the superagonistic agents (i.e. agents binding to the unmutated protein but not the mutated protein, should be superagonistic).

Table 1

CD28 family superagonistic epitopes
Epitopes are named according to the strands from which they derive.

	ප	NGTITHV	NGTQIYV TGGYLHI		
		TDIYFC	TGLYIC		
•	Ħ	FVION	LTIQG		
	د اق	SICONDOMY STATES	VISKI OF NO. 20 VSIKSLKFCHS		agonistic epitopes
		22	SIJKGLDSAVEVCV TVLRQADSQVTEVCA QLLKGGQILCD		PD-1 and BTLA superagonistic epitopes
		В	AVNLS GIASFV GVOIL		
	•	Α'	SPMLV PAVVL VEMEI		
		Protein	hCD28 hCTLA-4	IIICOS	· · · · · · · · · · · · · · · · · · ·

TDAFT	TTLYVT
F	NDNGSY
E	MSVVR
C';-D	QPGQDCRFR QTSWK
Ċ.C.	RMSPSNQTDK KLNG
B	DNATF
	PALLVV QSEHSI
	Protein hPD-1 hBTLA

Table 3

		•			•	
	Sequence	GNYSQQLQVYSKTGF	YMMGNELTFLDDS	KTKGSGNTVSIKSLK	LAAFPEDRSQPGQDCR	
	in		A-4	v.		•
•	Protein	hCD28	hCTLA-4	PICOS	hPD-1	
	•			٠		
	:	. •			:	

Table 2
Targets of inhibitory superagonist antibodies

Receptor	Chromosome	Expression	no. of ITIMs
r-niin	1q23-24	B, myeloid, mast	1
FcRIIB	7g22	Myeloid	2
PILR		В	2
CD72	· 9p	T, subset B	. 1
CD5	11q13	Myeloid, mast, NK	1
MAFA	12p12-13	NK, T	2
NKG2A	12p13.1-13.2	Myeloid, etc	1.
CD31	17q23	•	3
CMRF35H	17q24	Leukocytes	. 4
CD22	19q13.1	B	2
CD66a	19q13.2	Granulocytes, etc	. 1
CD66d	19q13.2	Granulocytes	1
CD33	19q13.3	Myeloid	1
SIGLEC5	19q13.3	Myeloid	1
SIGLEC6	19q13.3	B cells, myeloid	
SIGLEC7	19q13.3	NK, myeloid, etc	
ILT2,3,4,5	19q13.4	Myeloid, B, etc	4
LIR8	19q13.4	Myeloid, B, etc	. 4 .
LAIR-1	19q13.4	Leukocytes	· 2
	19q13.4	NK, T	2
KIR2DL	19q13.4	NK, T	2
KIR3DL SIRP	20p13	Myeloid, etc	2

Table 4

Co-ordinates of the CD28/5.11A1 crystal structure

REMARK							28_all	/xp	lor/ref1	L8/pos	itional	13.pdb"
REMARK	R=0	.2510	35 ·£	rom 25		. <b>7</b>		. :				•
REMARK	DATE:	)9-Ja	n-04	09:48					y user:			
ATOM	. 1		ASP	1.		22.280			.38.327		64.18	L
ATOM	2	CG	ASP	1		23.319			37.463		67.78	L.
ATOM	3	OD1	ASP	1		22.934			36.470		66.82	<b>L</b> `
MOTA	4	OD2	ASP	1	12	24.524			37.779		54.04	Ĺ
ATOM	5	·C	ASP	.1	_ 13	22.104			38.005		50.51	L
ATOM	6	o.	ASP	1	13	22.541			37.163		41.52	<b>L</b> .
MOTA .	. 7	N.	ASP	1	13	21.674			36.112		37.53	L
MOTA	, 8	CA	ASP	1.	, 13	21.547			37.579	-	50.29	. L
MOTA	9	N	ILE	. 2	13	22.073	••		39.314		51.24	
MOTA	10	CA .	ILE	2		22.567			39.890		50.84	. L
ATOM .	11	CB	ILE	2	1:	21.842	54.0	94	41.240		22.62	L
MOTA	. 12	ĊG2	ILE	2		22.278			41.781		18.55	
MOTA	13	CG1	ILE	2			54.0	•		•	30.61	L
MOTA	14 .	CD1	ILB	2	1	19.510	54.5	21	42.229		31.86	L
ATOM	15 ·	С	ILE	.3	1	24.086	53.7	14	40.119		54.91	, L
MOTA	. 16	0	ILE	.2	1	24.645	52.6	30	40.283		55.68	L
ATOM	17	N	GLN	3	` 1	24.749	54.8	69	40.136		58.93	L
ATOM	18	CA	GLN	3	. 1	26.204	54.9	23	40.322		56.95	L
ATOM	19	CB	GLN	3	. 1	26.847	7 55.6	79	39.145		60.02	
ATOM	. 20	CG	GLN	. 3 .	1	27.010	54.8	51	37.863		63.51	L
ATOM	21	CD	GLN	3	1	26.479	55.5	52	36.615	•	65.36	L
ATOM	22	OE1	GLN	3	1	27.024	1 56.5	68	36.174	1.00		
MOTA	23	NE2	GLN	.3	` 1	25.412	.55.0	03	36.038			L
ATOM	24	C	GLN	3	٠1	26.635	5 55.5	64	41.650	1.00	51.69	L
ATOM	25	0	GLN	3	1	26.179	9 56.6	49	42.004	1.00	54.63	L
ATOM	26	. N	MET	4	. 1	27.522	2 54.8	189	42.376		42.42	L
ATOM	27	CA	MET	4	. 1	28.005	5 55.3	92	43.660		37.64	L
MOTA	. 28	CB	MET	· 4	1	28.066	5 54.2	48	44.671		54.55	. <b>L</b>
MOTA	29	CG	MET	4	. 1	27.03	7 54.3	19	45.783		56.74	. <b>L</b>
MOTA	30	SD.	MET	4	1	25.360	54.6	33	45.189		76.06	L
MOTA	31	CE	MET	4	. 1	25.083	3 ,56.2	69	45.843		68.01	L
ATOM	32	C	MET	4	_ 1	29.39	2 56.0	800	43.507		44.16	· r
MOTA	33	0	MET	. 4	` 1	30.35			43.176		35.72	L
MOTA	34	N.	ASN	<b>5</b> ,	1	29.49			43.750		50.40	L
ATOM	· 35	CA	ASN	5	1	30.77	9 57.9	96	43.624		58.90	. L
MOTA	36	CB	ASN	5	1	30.70					67.94	. L
MOTA	37	CG	asn	5		30.11			41.233		59.91	, <b>r</b>
MOTA	38	OD1	· ASN	5	. 1	.30.78			40.474		49.08	L
ATOM	39	ND2	asn	5	. 1	.28.84			40.981		56.43	L
ATOM	40	C	ASN	5	1	.31.19	1 58.	543	44.939		46.55	L -
MOTA	41	0	ASN	5 .	. 1	30.61			45.368	•	40.94	L
MOTA	. 42	N	GLN	6		.32.20			45.577		33.77	L
ATOM	43	CA	GLN	, 6		.32.66			46.846		36.85	. L
ATOM	44	CB	GLN	6	1	.33.25	7 57.4	176	47.679	•	24.74	ŗ
ATOM	45	CG	GLN	6		32.39				·	19.84	L
ATOM	.46	, CD .	GLN	, 6	3	.32.39	3 55.	524	49.029	1.00	27.56	L

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L
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                                    132.925
                                               56.048
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ATOM
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                                               54.339
                                    131.803
               NE2
                    GLN
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                                                61.798
                                      144.534
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                      SER
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  ATOM
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                                                                   1.00 46.48
                                                         56.928
                                                62.894
                                      144.226
                      SER
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            89
                 0
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                                                         58.696 . 1.00 31.39
                                                                                     L
                                      144.519
                                                61.546
                      ALA
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                                                          59:666
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                                      144.116
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                      ALA
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            91.
  MOTA
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                                                          59.753
                                                                   1.00 28.98
                                                 62.610
                                      142.615
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  MOTA
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                                      144.706
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            93
                 C
                      ALA
  ATOM
                                                                   1.00 41.17
                                                          61.268
                                                 61.002
                                      144.928
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                      ALA
  MOTA
             94
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                                                 63,156
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                                      144.946
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            95
  MOTA
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                                                                   1.00 42.50
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                                      145.553
                                                 62.865
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                 CA
                      SER
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                                                 64.012
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  MOTA
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                                                 63.522
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  MOTA
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                                                 62.553
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64.217
                                              62.586
                                    143.395
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ATOM
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                            32
               CD2
 MOTA
          233
                                                                 1.00 36.20
                                                                                   L
                                                        51.597
                                              54.493
                                    113.571
                             32
                    TRP
          234
               CE2
 MOTA
                                                                 1.00 25.93
                                                                                   L
                                                        52.798
                                              53.149
                                    115.183
                             32
               CE3
                    ם פייני
          235
 MOTA
                                                                                   L
                                                                 1.00 47.52
                                               55.074
                                                        49.765
                                    114.706
                CD1 TRP
                             32
          236
MOTA
                                                                                   L
                                                                 1.00 36.87
                                                        50.418
                                    113.504
                                               55.193
               NE1 TRP
                             32
          237
 ATOM
                                                                                   L
                                                                 1.00 25.25
                                                        52.591
                                               54.319
                                    112.610
                             32
                CZ2 TRP
 ATOM
          238
                                                                                   L
                                                                 1.00 21.98
                                                        53.788
                                    114.229
                                               52.978
                    TRP
                             32
                CZ3
          239
 ATOM
                                                                                   L
                                                                       2.00
                                                                 1.00
                                                        53.677
                                               53.563
                                   . 112.954
                             32
          240
                CH2 TRP
 MOTA
                                                                 1:00 17.38
                                                                                   L
                                                        50.645
                                               54.578
                                    119.419
                             32
                C
                     TRP
          241
 ATOM
                                                                                   L
                                                                 1.00 20.83
                                               54.267
                                                        49.491
                                     119.697
                             32
                0
                     TRP
          242
 MOTA
                                                                                    L
                                                                 1.00 19.97
                                               54.750
                                                        51.599
                                     120.332
                             33
                N.
                     LEU
          243
 MOTA
                                                                                    L
                                                                 1.00 39.54
                                                        51.357
                                               54.570
                                     121.763
                             33.
                     LEU
          244
                CA
 ATOM
                                                                 1.00 44.19
                                                                                    L
                                               55.790
                                                        50.642
                                     122.352
                             33
          245
                CB
                     LEU
 MOTA
                                                                 1.00 34.32
                                                                                    L
                                                        50.500
                                               55,803
                                     123.876
                             33
                     LEU
                CG
 ATOM
          246
                                                                                    L
                                                                 1.00 27.47
                                                        49.078
                                               56.190
                                     124.252
                             33
                CD1
                    LEU
          247
 ATOM
                                                                                    L
                                                                  1.00 19.98
                                                        51.515
                                               56.774
                                     124.479
                             33
                CD2
                     LEU
          2.48
 MOTA
                                                                  1.00 39.15
                                                                                    L
                                                        52.685
                                     122.481
                                               54.371
                             33
                C
                     LEU
           249
 MOTA
                                                                                    L
                                                                  1.00 42.09
                                                        53.595
                                               55.182
                                     122.345
                             33
           250
                0
                     LEU
  MOTA
                                                                                    L
                                                                  1.00 38.96
                                                        52.785
                                               53.303
                                     123.262
           251
                N
                     ASN
                             34
  ATOM
                                                                                    L
                                                        54.017
                                                                  1.00.33.81
                                               53.008
                                     123.969
                     ASN
                             34
           252
                 CA
  MOTA
                                                                                    L
                                                                  1.00 29.67
                                                        54.470
                                     123.635
                                               51.588
           253
                 CB
                     ASN.
                             34
  MOTA
                                                                  1.00 18.96
                                                         53.908
                                                51.104
                                     122.323
                 CG
                     ASN
                             34
           254
  MOTA
                                                                                    L
                                                                 1.00 22.09
                                                         54.384
                                                51.484
                                     121.252
                             34
                 OD1
                     ASN
           255
  MOTA
                                                                                    L
                                                                  1.00 22.68
                                                         52.883
                                                50.269
                                     122.396
                             34
                ND2
                     ASN
           .256
  MOTA
                                                         53.889 . 1.00 27.35
                                     125.465.
                                                53.162
           257.
                 C
                     ASN
                             34.
  MOTA
                                                                  1.00
                                                         52.785
                                                53.215
                                      125.996
                              34
                     ASN
  MOTA
           258
                 0
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1.00 31.00
                                                      55.041
                                   126.125
                                             53.242
                   TRP
                           35
ATOM
         259
              N
                                                                                  L
                                                                1.00
                                                                     37.04
                                                      55.122
                                            ;53.380
                                   127.574
                           35
              CA
                   TRP
         260
MOTA
                                                                1.00 44.59
                                                      55.871
                                             .54.663
                                   127.942
                           35
                   TRP
         261
              CB
MOTA
                                                                1.00 50.73
                                                                                  L
                                                      55.099
                                             55.956
                                   127.725
                           35
                   TRP
              CG
         262
ATOM
                                                                                  L
                                                                1.00 39.25
                                                      54.155
                                   128.624
                                             56.560
                           35
                   TRP
              CD2
         263
MOTA
                                                                                  L
                                                                1.00 36.81
                                                       53.738
                                   128.042
                                              57.776
               CE2
                   TRP
                           35
         264
MOTA
                                                                                  L
                                                       53.621
                                                                1.00 29:95
                                              56.194
                                   129.868
                           35
         265
               CE3
                   TRP
MOTA
                                                       55.208
                                                                1.00 38.58
                                                                                  L
                                   126.660
                                             56.808
         266
               CD1
                   TRP
                           35
ATOM
                                                                1.00 40.14
                                                                                  L
                                                       54.397
                                              57.900
                                   126.843
                           35
         267
               NE1
                   .TRP
ATOM
                                                                1.00 .36.05
                                                       52.812
                                                                                  L
                                              58.629
                                   128.655
                           35
                   TRP
         268
               CZ2
ATOM.
                                                       52.698
                                                                1.00 39.51
                                              57.045
                                    130.479
                   TRP
                           35
         269
               CZ3
MOTA
                                                                1.00 31.94
                                                       52,307
                                              58.247
                                    129.871
                           35
         270
               CH2
                   TRP
ATOM
                                                                1.00 32.85
                                                                                  L
                                                       55.885
                                    128.118
                                              52.168
                            35
                    TRP
         271
               С
ATOM
                                                      56.849
                                                                1.00 24.56
                                                                                  L
                                              51.715
                                    127.499
                            35
               0
                    TRP
         272
MOTA
                                                                                  L
                                              51.654
                                                       55.451
                                                                1.00 29.03
                                    129.271
                          ∵ 36
               N
                    TYR
         273
ATOM
                                              50.488 56.080
                                                                1.00 24.01
                                    129.894
                            36
               CA
                    TYR
ATOM
         274
                                                                1.00 24.57
                                              49.256
                                                       55.178
                                    129.760
                            36.
                    TYR
MOTA
         275
               CB
                                                                                   L
                                                                1.00 36.78
                                                       54.845
                                              48.844
                                    128.341
                            36
                    TYR
         .276
               CG
ATOM
                                                                1.00 45.66
                                                                                   L
                                                       55.469
                                              47.745
                                    127.740
                            36
                    TYR
         277
               CD1
ATOM
                                                                1.00 29.26
                                                                                   L
                                              47.350
                                                       55.138
                                    126.439
                    TYR
                            36
               CE1
MOTA
         278
                                                                 1.00 43.28
                                                                                   L
                                              49.536
                                                       53.885
                                    127.606
                            36
               CD2
                    TYR
MOTA
         279
                                                                 1.00 29.25
                                                                                   L
                                                       53.550
                                    126.314
                                              49.153
                    TYR
                            36
         280
               CE2
MOTA'
                                                                 1.00 33.13
                                                                                   L
                                                       54.174
                                              48.064.
                            36
                                    125.736
                    TYR
               CZ
 MOTA
          281
                                                                 1.00 29.39
                                                                                   L
                                                        53.810
                                              47.709
                                    124.458
                            36
                    TYR
               OH
          282
 ATOM
                                                                                   Ţ,
                                                                 1.00 34.79
                                              50.683
                                                        56.401
                                    131.379
                            36
               C
                    TYR
          283
 ATOM
                                                                                  · L
                                                                 1.00 31.84
                                                        55.813
                                              51.530
                                    132.060
                            36
               0
                    TÝR
 ATOM-
          284
                                                                                   L
                                                                 1.00 38.75
                                                        57.337
                                               49.880
                                    131.876
         285
               ·N
                    GLN
                            37
 ATOM
                                                                                   L
                                                                 1.00 41.58
                                                        57.731
                                              49.923
                                    133.278
                            37
                    GLN
          286
                CA
 ATOM
                                                                 1.00 30.71
                                                        59,199
                                               50.342
                                    133.406
                    GLN
                            37
          287
                CB
 ATOM
                                                                 1.00, 37, 19
                                                        59.704
                                               50.495
                                     134.852
                            37
          288
                CG
                    GLN
 MOTA
                                                                 1.00 25.39
                                                        61.222
                                               50.332
                                     134.989
                             37
                CD
                    GLN
          28.9
 ATOM
                                                                 1.00 36.25
                                                        61.753
                                     134.904
                                               49.222
                             37
                OE1
                    GLN
          290
 ATOM
                                                                 1.00 22.58
                                                        61.918
                                               51.439
                             37
                                     135.209
                    GLN
          291
                NE2
 ATOM
                                                                                    L
                                                                 1.00 39.79
                                                        57.528
                                               48.528
                             37
                                     133.884
          292
                C
                    GLN
 ATOM
                                                                 1.00 29.52
                                                                                    L
                                                        57.975
                                               47.526
                                     133.319
                    GLN
                             37.
                0
          293
 ATOM
                                                                1.00 29.65
                                                                                    L
                                                        56.839
                                               48.465
                                    135.022
                    GLN
                             38
                N
          294
 MOTA
                                                                                    Ь
                                                                 1.00 31.00
                                               47.195
                                                        56.596
                                     135.695
                    GLN
                             38
          295
                CA
 MOTA
                                                                                    L
                                                        55.155
                                                                 1.00 37.06
                                               46.738
                                     135.471
                             38
          296
                CB
                     GLN
 MOTA
                                                                                    L
                                                                 1.00 37.85
                                                        54.724
                                               45.597
                                     136.385
                     GLN
                             38
          297
                CG
 MOTA
                                                                                    L
                                                                 1.00 51.91
                                                        53.401
                                              44.992
                                     135.973
                     GLN
                             38
          298
                CD
 ATOM
                                                                                    L
                                                                  1.00 56.78
                                                        52.399
                                               45.693
                                     135.856
                     GLN
                             38
           299-
                OE1
 ATOM
                                                                                    L
                                                                  1.00 47.92
                                                        53.390
                                               43.683
                                     135.753
                             38
           300
                NE<sub>2</sub>
                     GLN
 MOTA
                                                                  1.00 23.61
                                                         56.860
                                               47.285
                                     137.192
                             38
                C
                     GLN
           301
 ATOM
                                                                                    L
                                                                 1.00 30.06
                                               47.630
                                                         55.963
                             38
                                     137.952
                0
                     GLN
 MOTA
           3.02
                                                                                    L
                                                                  1.00 29.96
                                               46.969
                                                         58.086
                                     137.610
                             39
          303
                N
                     LYS
 ATOM
                                                                                    L
                                                                  1.00 20.79
                                                47.022
                                                         58.464
                                     139.021
                             39
                     LYS
           3'04
                CA
 MOTA
                                                                                    L
                                                                  1.00 26.60
                                                46.606
                                                        .59,925
                                     139.204
                             39
           305
                CB
                     LYS
  ATOM
                                                                                    L
                                                                  1.00 31.56
                                     139.493
                                                         60.884
                                               47.764
                             39
                CG
                     LYS
  ATOM
           306
                                                                                    L
                                                                  1.00 24.64
                                     138.268
                                               48.135
                                                         61.727
                     LYS
                             39
                 CD
           307
  MOTA
                                                                                    L
                                                                  1.00 28.08
                                     138.633
                                                48.266
                                                         63.205
                             39
                 CE
                     LYS
           308
  ATOM
                                                                                    L
                                                                  1.00 32.42
                                     137.922
                                                47.293 .64.094
                             39
                NZ
                     LYS
           309
  MOTA
                                                                                     L
                                                                  1.00 39.66
                                                         57.566
                                                46.103
                             39
                                     139.831
                 C
                     LYS
           310
  MOTA
                                                                  1.00 49.56
                                                         56.886
                                     139.272
                                                45.238
                             39
                 O
                     LYS
           311
  ATOM
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			•					1.00 54.59	L
MOTA	312	N	PRO	40	141.161	46.283	57.533	1.00 52.22	···L
MOTA	·313	CD	PRO	40	141.957	47.289	58.266	1.00 52.22	Ŀ
ATOM	314	CA	PRO.	40 .	142.007	45.434	56.686	1.00 40.87	L
MOTA	315	CB	PRO '	· 40	143.431	45.874	57.037		. L
ATOM	316	CG	PRO.	40	143.274	47.280	57.530	1.00 36.77	. L
ATOM	317	C	PRO	40	141.792	43.935	56.895	1.00 53.33	
MOTA	318	0	PRO	4.0	141.962	43.429		1.00 48.18	L
ATOM	319	N	GĽÝ	41	141.403	43.244	55.825	1.00 56.47	. <b>L</b>
ATOM	320	·CA	GLY	. 41	141.178	41.807	55.889 <sub>.</sub>	1.00 46.36	L
ATOM	321	C.	GLY	41	140.030	.41.378 -		1.00 47.51	L
MOTA	322	ο.	GLY	41	139.890	40.195	57.103	1.00 42.82	· L
MOTA	323	N	ASN ·	.42	139.198	42.336	57.· <b>177</b>	1.00.39.14	Ĺ
MOTA	324	CA	ASN	42	138.061	42.049	58.044	1.00 33.16	L
MOTA	325	CB	ASN	42	138.031	43.041	59.210	1.00 25.23	L
ATOM	326	CG	ASN	42	137.400	42.453	60.451	1.00 34.65	L
	327		ASN	. 42	136.876	41.338	60.416	1.00 42.65	L
ATOM	.328		ASN	42	137.444	43.194	61.558	1.00 15.22	L
ATOM	.328 ;329	C	ASN	42	136.743	42.123	57.287	1.00 36.43	L
ATOM	-	0	ASN	42	136.726	42.413	56.092	1.00 31.10	. <b>L</b>
ATOM	330	•	ILE	.43	135.648	41.852	57.993	1.00 46.04	L
MOTA	.331	N CA	ILE	43	134.310	41.894	57.407	1.00 55.78	, <b>L</b>
MOTA	332		ILE	43	133.340	40.879	58.089	1.00 55.57	· L
MOTA	333	CB		43	134.038	39.554	58.323	1.00 47.83	L
MOTA	334	CG2	•	43	132.828	41.439	59.423	1.00 61.00	· L
MOTA .	335	CG1		43	131.656	40.662	60.017	1.00 6B.36	L
ATOM	336	CD1		43	133.726	43.298	57.555	1.00 63.83	· L
MOTA	337	C ·	ILE	43	134.037	44.010	58.513	1.00 72.13	. · L
MOTA	. 338	0	ILE	44	132.881	43.720	56.605	1.00 56.85	L
MOTA	33.9	N	PRO	44	132.444		55.402	1.00.59.76	P
MOTA	340	CD	PRO	44	132.282	45.052	56.681	1.00 47.82	Ľ.
ATOM	. 341	CA	PRO	44	131.893	45.349	55.242	1.00 52.95	L.
ATOM	342	CB	PRO	44	131.590		54.665	1.00 66.17	L
MOTA	343	CG	PRO	44	131.079	45.064	57.613	1.00 41.70	L
MOTA	344	C,	PRO	44	130.160	44.258	57.460	1.00 35.22	L
MOTA	345	0	PRO		131.095	45.982	58.575	1.00 33.96	L
ATOM	346	И	LYS	. 45	130.010	46.106	59:537	1.00 39.65	L
MOTA	347	CA	LYS	45	130.576		60.953	1.00 36.05	L
MOTA	348	CB	LYS	45	132.096	_	61.012	1.00 44.96	L
MOTA	349	CG	LYS	45	132.651		61.752	1.00 53.54	L
MOTA	350	CD	LYS	. 45	134.060			1.00 58.35	L'
MOTA	351	CE	LYS	45. ·	134.818		62.586	1.00 46.04	L
MOTA	352	NZ	LYS	45	129.162		59.218	1.00 37.07	L
MOTA	3:53	C	LYS	45	129.686		58.817	1.00 37.21	, L
MOTA	3.54		LYS	45	127.850		59.385	1.00 22.26	L
MOTA	355		LEU	46		48.326		10	, L
ATOM	3.56		LEU	46	125.505				L
MOTA	357		LEU	46	•	_			L
MOTA	. 358			46	124.429				
MOTA	359		1 LEU		123.264				· Li
MOTA	360		2 LEU	46	124.987				L
MOTA	361		LEU	46	127.268				L
MOTA	362		LEU	46	127.353				L
MOTA	. 363		LEU	47	127.414				L
ATOM	364	. CA	LEU	47	127.719		90.302		
				•	•	٠.			

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ATOM	365	CB	LEU	47	128.915	52.562	59.755	1.00 25.09	. · L
ATOM	366	CG	LEU	47 .·	130.100	52.926	60.636	1.00 16.21	· . L
ATOM	367	CD1	LEU	47	130.727	51.676	61.198	1.00 17.63	Li
ATOM	368	CD2	LEU.	47	.131.094	53.701	59.805	1.00 2.00	. L
ATOM	369	С	LEU	47	126.535		60.449	1.00 34.89	L
ATOM	370	0.,	LEU	47	126.190	53.282	61.535	1.00 26.31	L
ATOM .	371	N	ILE	· 48	125.934	53.100	59.293	1.00 44.65	L
ATOM	372	CA	ILE	48	124.794	54.018	59.187	1.00 34.33	Ŀ
ATOM	373	CB	ILE	48	125.251	55.439	58.788	1.00 24.64	L
ATOM	374		ILE	48	124.145	56.146	58.008	1.00 29:43	L
ATOM	375	CG1		48	125.591	56.253	60.033	1.00 28.98	L.
ATOM	376		ILE		126.967	56.866	59.993	100 25.03	L
ATOM	377 :		ILE	48	123.775	53.576	58.133	1.00 29.31	L
ATOM	.378	0	ILE	48	124.113	53.411	56.962	1.00 40.59	. L
ATOM .	. 379		·TYR	49	122.527	53.405	58.547	1.00 15.91	L
ATOM	380	CA	TYR	49 .	121.485	53.018	57.613	1.00 21.27	L.
MOTA	.381	CB	TYR	49	120.762	51.748	58.087	1.00 36.34	L
	382	CG	TYR	49	119.779	51.925	59.231	1.00 35.16	· L
MOTA.	.383		TYR	49	118.408	52.066	58.986	1.00.25.01	, L
MOTA				49	117.498	52.216	60.028	1.00 28.72	L
ATOM .	.384	CD2	TYR	49	120.214	51.934	60.560	1.00 28.85	L
ATOM	385	CE2		49	119.308	52.084	61.614	1.00 30.37	L
ATOM ·	386		TYR	49	. 117.953	52.228	61.340		L
MOTA	387	CZ OH	TYR	49	117.048	52.410	62.370	1.00 55.09	L
ATOM	388		TYR	49	120.510	54.172	57.486	1.00 24.72	L
MOTA	389	C		4.9	120.310	55.037	58.356	1.00 26.69	L
ATOM	390	0	TYR LYS	50 ·	119.762	54.189	56.392	1.00 25.34	L
ATOM	391	N		50	118.786	55.241	56.132	1.00 19.61	· L
MOTA	·392	CA	LYS	50 . 50	117.611	55.134	57.108	1.00 42.59	L
MOTA	393	CB	LYS	50	116.426	54.345	56.566	1.00 36.91	· L
ATOM	394	. CG	LYS	50 50	115.124	55.118	56.723	1.00 40.28	L
ATOM .	395	CD	LYS		114.289	54.568	57.865	1.00 33.03	L
MOTA	396	CE	LYS		112.829	54.799	57.659	1.00 38.05	L
MOTA	397	NZ	LYS	50 50	119.368	56.645	56.192	1.00 22.01	L
MOTA	398	C	LYS	. 50	119.383	57.575	56.623	1.00 30.12	L
MOTA	399	0	LYS	50	120.622	56.790	55.779	1.00 32.92	. L
MOTA	400	N	ALA	51	121.275	•	55.749	1.00 27.76	. L
MOTA	401	CA	ALA	51		. 59.117	55.100		L
ATOM	402	CB	ALA	51 51	120.346 121.787		57.073	1.00 25.18	L
MOTA	403	C.	ALA	51 51	122.949	59.026	57.173	1.00 28.58	L
MOTA.	404	0.	ALA	. 51	120.927	58.714	58.081	1.00 22.15	. L
MOTA	405	N	SER	52	121.347		59.362	1.00 19.39	L
MOTA	406	CA	SER	52	•			1.00 25.09	L
ATOM	407	CB	SER	52 -	120.690		58.390	1.00 53.81	. <b>T</b>
ATOM	408		SER	52	120.199	58.369	60.518	1.00 20.68	L
ATOM	409	C	SER	52	121.021	58.729	61.674	1.00 23.62	L
MOTA	410	0	SER	52	121.232	57.194	60.209	1.00 25.87	L
ATOM	411	N	ASN	53 53	120.497		61.254	1.00 27.39	Ŀ
MOTA	412	CA	ASN	53	120.157	55.387	60.811	1.00 27.53	L
MOTA	413	CB	ASN	53	118.992	55.895	61.323	1.00 27.34	L
MOTA	414	CG	ASN	53	117.668	55.656	60.729	1.00 26.55	L
MOTA	415		ASN	, 53	116.619	56.607	62.450	1.00 36.37	L
MOŢA	416		ASN	53	117.713	55.402	61.592	1.00 35.37	· L
MOTA	417	С	ASN	53	121.366	JJ.402	V = 1 3 2 4	1,00 20,27	
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1.00 34.60
                                                       60.783
                                    121.809
                                              54.592
               O
                   ASN
         418
MOTA
                                                                1.00 34.99
                                                       62.795
                                    121.899
                                              55.607
                   LEU
         419
               N
MOTA
                                                                 1.00 47.12
                                                                                   L
                                    123.064
                                              54.880
                                                       63.294
                   LEU
                            54
               CA
ATOM
         420
                                                                                   T,
                                                       64.510
                                                                 1.00:37.02
                                    123.649
                                              55.607
                   LEU
               CB
         421
MOTA
                                                                 1.00 20.40
                                              .55.873
                                                       64.594
                                    125.152
                   LEU
                            54
               CG
MOTA
          422
                                                                                   L
                                                       63.830
                                                                1.00 25.30
                                    125.508
                                              57.117
                            54.
               CD1 · LEU
ATOM
          423
                                                                 1.00 22.53
                                                                                   L
                                                       66.039
                                              56.034
                                    125.533
                            54
               CD2 LEU
          424
MOTA
                                                                 1.00 56.63
                                                        63.705
                                    122.660
                                              53.468
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               C
                    LEU
MOTA
          425
                                                                 1.00 68.94
                                                       64.145
                                              53.250 .
                                    121.529
                            54
               0
                    LEU
          426
. ATOM
                                                                                   L
                                                        63.573
                                                                 1.00 51.79
                                              52.513
                                    123.578
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               N
                    HIS
          427
 MOTA
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                                                                 1.00 38.57
                                                        63.948
                                               51.142
                                    123.267
                            55
          428
               CA
                    HIS
 ATOM
                                                                 1.00 36.54
                                                                                   L
                                                        63.137
                                    124.091
                                              50.13.9
                    HIS
                            55
               CB
          429
 MOTA
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                                                                 1.00 27.93
                                                        63.186
                                               48.742
                                    123.551
               CG
                    HIS
                            55
          430
 MOTA
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                                                                 1.00 31.02
                                                        63.551
                                    122.338
                                               48.268
                            55
               CD2
                   HIS
          431
 MOTA
                                                                                    L
                                                                 1.00 36.74
                                                      . 62.841
                                               47.639
                                    124.303
                    HIS
                            55
          432
               ND1
 MOTA
                                                                                    L
                                                                 1.00 43.03
                                              46.545
                                                        62.993
                                    123.573
                            55
          433
                CE1 HIS
 MOTA
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                                                                 1.00 37.77
                                               46.902
                                                        63.423
                                     122.376
                            55
                NE2 HIS
          434
 MOTA
                                                                                    L
                                                                 1.00 38.01
                                               50.925 - 65.424
                                     123.513
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                    HIS
                C
          435
 MOTA
                                                                 1.00 47.97
                                               51.634: 66.058
                                     124.296
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 MOTA
                                                                 1.00 33.15
                                                                                    L
                                                      .65.966
                                               49.930
                             56
                                     122.832
                N
                    THR
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 MOTA
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                                                        67.371
                                               49.600
                            .56
                                     122.951
                    THR
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                CA
 ATOM
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                                                                 1.00 58.72
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                             56
                CB
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                                                                  1:00 57.81
                                                        66.495
                                               47.787
                                     121.601
                    THR
                             56
                OG1
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 ATOM.
                                                                  1.00 63.75
                                                                                    L
                                                        68.430
                                     120.770
                                               48.955
                             56
          441
                CG2
                     THR
 ATOM
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                                                        67.805
                                                                 1.00
                                                                       32.47
                                               49.260
                                     124.380
                             56
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                C
                     THR
 ATOM
                                                        67.415
                                                                  1.00 23.36
                                               48.236
                                     124.940
                     THR
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 ATOM
                                                                 1.00 28.03
                                                        68.612
                                     124.967
                                               50.136
                     GLY
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 ATOM
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                                               49.893
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                             57
                CA ·
                     GLY
           445
  MOTA
                                                                  1.00 48.73
                                                         68.403
                                               50.703
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                     GLY
           446
                C
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                                                                  1.00 45.48
                                                         68.641
                                               50.506
                                     128.584
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                     GLY
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  ATOM
                                                                  1.00 45.32
                                               51.616
                                                         67.537
                                     126.971
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                N
           448
  MOTA
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                                               52.439
                                                         66.819
                                     127.926
                     VAL
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                CA
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                CG1
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                                                53.768
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  MOTA
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                                                         67.780
                                                54.509
                                      127.178
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                      VAL
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  ATOM
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                                                                  1.00 38.91
                                                         67.951
                                      129:378
                                                54.059
                              59
           455
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                     PRO
  MOTA
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                                                                  1.00 42.54
                                                         67.788
                                                53.187
                                      130.553
                              59
                     PRO
         . 456
                 CD
  MOTA
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                                                                   1.00 38.07
                                                         68.658
                                                55.296
                                      129.717
                      PRO
                              59
                 CA
           457
                                                                                     L
  ATOM
                                                                   1.00 34.29
                                                         68.706
                                                55.289
                                      131.253
                              59
                 CB
                      PRO
           45B
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  MOTA
                                                                   1.00 25.37
                                                         67.847
                                                54.148
                                      131.698
                              59
                      PRO
           459
                 CG
  MOTA
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                                                                   1.00 36.88
                                                         67.980
                                                56.543
                                      129.174
                              59
                 C
                      PRO
           460
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                                                                   1.00 38.73
                                                56.694
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                                      129.273
                              59
                      PRO
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           461
  MOTA
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                                                         68.782
                                                57.437
                                      128.605
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           462
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  MOTA
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                                                                   1.00 37.70
                                                          68.274
                                                58.680
                      SER
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                                      128.044
                 CA
            463
   MOTA
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                                                                   1.00 47.02
                                                          69.424
                                                59.513
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            464
   ATOM
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                                                          70.648
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                                      128.108
                , OG.
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            465
   ATOM
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                                                          67.536
                                                 59.492
                                      129.096
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   ATOM-
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                                                                   1.00 38.05
                                                          66.785
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            467
   MOTA
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                                                          67.758
                                                                   1.00 31.36
                                                 59.175
                                      130.369
                      ARG
                              61
                 N
   ATOM
            468
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                                                                   1.00 40.37
                                                 59.887
                                                          67.068
                                      131.440
                 CA
                      ARG
                               61
            469
  ATOM
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                                                                   1:00
                                                 59.241
                                                          67.361
                                       132.801
                               61
                  CB
                      ARG
            470
   MOTA
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ATOM	471	CG	ARG	61	133.316	58.277	66.278	1.00 55.44	L
MOTA	472	CD.	ARG	61	134.854	58.263	66.188		L
ATOM	473	NE	ARG	61	135.482	57.895	67.458	1.00 41.22	L
ATOM	474	CZ	ARG	61	135.733	56.646	67.834	1,00 36.39	L
ATOM	475	NH1	ARG	61	135.411	55.637	67.041	1.00 46.50	
ATOM	476	NH2	ARG	61	136.294		69.008	1.00 45.10	. L
ATOM	477	c ·	ARG	61	131.137	59.822	65.573	1.00 39.44	r L
ATOM	478	0	ARG	61	131.495	60.718		1.00 31.59	L
ATOM	479	N	PHE	62	130.468	58.744	65.176	1.00 29.20	L
ATOM	480	CA:	PHE	62	130.083	.58.534	63.795	1.00 21.62	L
ATOM	481	CB	PHE	62	129.922	57.038	63.507	1.00 15.95	L
ATOM	482	CG	. PHE	62 ·	131.216	56.325	63.248	1.00 28.60	L
ATOM	483	CD1	PHE	62	131.770	56.303	61.975	1.00 25.81	L
ATOM	484		PHE	62	131.884	55.661	64.277	1.00 34.71	ь
ATOM		·CE1		62	132.973	55.629	61.730	1.00 25.28	L
ATOM	486	CE2	PHE	62	133.086	54.987	64.039	1.00 17.13	ŗ
ATOM	487	CZ .	PHE	62	133.628	54.972	62.759	1.00 16.17	, r
MOTA	488	c ·	PHE	62	128.749	59.223	63.574	1.00 27.58	. <b>L</b> .
ATOM	489	0	PHE	62	127.812	59.041	64.347	1.00 26.02	L
ATOM	490	N	SER	63	128.667	60.028	62.526	1.00 27.01	L
ATOM	491	CA	SER	63	127.432	60.724	62.194	1.00 29.21	L
MOTA	492	CB	SER	63	127.512	62.197	62.620	1.00 27.06	L
ATOM	493	OG	SER	63	127.604	•	61.501	1.00 46.67	L
ATOM	494	C	SER	63	127.271	60.609	60.689	1.00 31.69	L.
MOTA	495	0	SER	63	128.247	60.359	59.983	1.00 35.00	L L
ATOM	496	, N	GLY	64	126.046	60.778	60.203	1.00 32.44	Li Li
MOTA	497	CA	GLY	64	125.796	60.677	58.775	1.00 28.03 1.00 36.15	· L
MOTA	498	С	$Gr\lambda$	64	. 124.656	61.567	58.325	1.00 38.15	L
MOTA	499	0	GLY	64	123.678	61.753	59.050	1.00 31.20	L.
MOTA	500	N	SER	. 65	124.761	62.103	57.115	1.00 43.47	ь.
MOTA	501	CA	SER	-65	123.723	62.993	56.612	1.00 43.04	L.
MOTA	502	CB	SER	65	124.029		57.075	1.00 39.28	
MOTA	503.	QG	SER	65·	125.378	64.487	57.510	1.00 49.79	L
ATOM	504	С	SER	65	123.566	62.975	55.097	1.00 35.77	· L
ATOM	505	0	SER	65	124.401	62.428	54.373 54.625	1.00 17.16	L
MOTA	506	N	GLY	66	122.485	63.579	53.196	1.00 29.10	L
MOTA	507	CA	GLY	66	122.258	63.641 63.081	52.769	1.00 35.42	· L
MOTA	508	C.	GLY	66	120.920	62.267	53.479	1.00 32.46	L
MOTA	509		GLY	66	120.321	63.527	51.608	1.00 24.62	L.
MOTA	510	И	SER	. 67	120.449 119.184	63.062	51.061	1.00 28.74	L
ATOM	511	CA	SER	67 67	118.012		51.757	1.00 46.75	L
MOTA	512	CB	SER	67	116.780	63.757	51.412	1.00 59.32	,L
MOTA	513	OG	SER	· 67	. 119.129	63.343	49.567	1.00 32.92	L
MOTA	514		SER	67 67	119.579		49.113	1.00 35.08	L
MOTA	515	0	SER	67 68	118.589	•	•	1.00 32.00	L
MOTA	`516	N	GLY		118.485				L
ATOM	517	CA		68 68	119.712				L
ATOM	518	C	GLY.	68	119.712				L
MOTA	. 519		GLY THR	69	120.567	·			L
MOTA	520	N		69	121.784				. <b>L</b>
MOTA	521	CA		. 69	121.890				L
MOTA	522	.CB OG		69	120.775	• -			L
MOTA	523	.00	TIUK	0,5					

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                                    123.175
              CG2
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                    THR
MOTA.
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                                                                       29.87
                                                        46.376
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MOTA
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                                                                      38.58
                                                        46.350
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ATOM
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                                    123.082
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                    GLY
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          527
MOTA
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                                                                 1.00 42.61
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                                    124.234
                    GLY
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ATOM
          528
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MOTA
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 ATOM
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 MOTA
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ATOM
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                CB
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                                                                 1.00 38.58
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                                                        50.263
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                             71
                CG
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 MOTA
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 MOTA
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                    PHE
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                                                                 1.00 26.37
                                               60.021
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                CEI
                    PHE
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                CE2
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 ATOM
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                     PHE
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 MOTA
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 MOTA
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                CA
 ATOM
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                                                                       32.81
                                                         53.781
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                             72
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 MOTA
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                                                                       56.77
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 MOTA
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  MOTA
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           5.51
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  MOTA
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                              73
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           552
                 CG
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  MOTA
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                                      129.287
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                     LEU
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  MOTA
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                                      131.586
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           554
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  ATOM
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                                                        . 58.567
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                                                          59.436
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                                      131.443 62.362
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                 OG1
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  MOTA
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                                                 64.524
                                                          60.747
                                      131.588
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                 CG<sub>2</sub>
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  ATOM
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  ATOM
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  MOTA
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            564
   MOTA
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                  CA
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   MOTA
            566
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                                                          62.847
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   MOTA
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                                                                    1.00 33.47
                                       133.988
                                                 58.479
                              75
                  CGl
                      ILE
            568
                                                                                      L
   MOTA
                                                                    1.00 25.94
                                                          59.687
                                       133.840
                                                 58.343
                               75
                      ILE
                  CD1
   MOTA
            569
                                                                                      L
                                                                    1.00 34.16
                                                          62.914
                                       134.399
                                                 61.855
                               75
                       ILE
                  C
            570
                                                                                      L
   ATOM
                                                                    1.00 28.63
                                                          62.537
                                                62.381
                               75
                                       135.440
                       ILE
                  0
   MOTA
            571
                                                                    1.00 42.00
                                                                                      L
                                                           64.059
                                                 62.167
                                       133.803
                               76
                  N
                       SER
            572
                                                                                      L
                                                                    1.00 51.91
   · ATOM
                                                           64.971
                                                 63.155
                                       134.366
                               76
                       SER
                  CA
                                                                                      L
            573
   ATOM
                                                                    1.00 67.85
                                                 63.762
                                                           65.829
                                       133.251
                               76
                       SER
                  CB
                                                                                      L
            574
   MOTA
                                                                    1.00 75.08
                                                           65.449
                                                 63.244
                                       131.981
                               76
                       SER
            575
                  OG
   MOTA
                                                                         55.79
                                                           65.865
                                                                    1.00
                                                  62.507
                               76
                                       135.424
                       SER
            576
                  C
   ATOM
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66.131
                                     135.372
                                               61.304
                    SER
                            76
          577
                0
MOTA
                                                        66.319
                                                                  1.00
                                                                       51.60
                                               63.307
                                    . 136.384
                            77
                N
                    SER
          578
ATOM
                                                                 1.00
                                                        67.177
                                                                       51.14
                                               62.818
                                     137.459
                            77
          579
                    SER
                CA
 МОТА
                                                                                    L
                                                                  1.00 51.40
                                                        68.633
                                     136.993
                                               62.788
                            77
                CB
                    SER
          580
 ATOM
                                                                                    L
                                                                  1:00 52.89
                                                         68.967
                                     136.336
                                               63.998
                            77
          581
                OG
                    SER
 MOTA
                                                                                    T.
                                                                  1.00 49.10
                                                        66.755
                                               61.433
                            77
                                     137.938
                C
                    SER
          582
 MOTA
                                                                                    L
                                                                  1.00 47.48
                                                         67.311
                                               60.422
                                     137.515
                             77
                     SER
          583
                0
 MOTA
                                                                                    L
                                                                  1.00 46.54
                                               61.406
                                                         65.771
                             78
                                     138.832
                     LEU
          584
                N
 ATOM
                                                                                    T.
                                                                  1.00 32.83
                                                         65.241
                                               60.168
                                     139.389
                             78
          585
                CA
                    LEU
 ATOM
                                                                                     L
                                                                  1.00 27.78
                                                        .64.084
                                               60.495
                                     140.333
                    LEU
                             78
          586
                CB
 MOTA
                                                                  1.00 35.44
                                                                                     L
                                                         62.950
                                                59.481
                                     140.423
                             78
                ÇG
                    LRU
          587
 MOTA
                                                                                     L
                                                                  1.00 40.91
                                                         61.855
                                                59.898
                                     139.472
                             78
                    LEU
          588
                CD1
 ATOM
                                                                  1.00 25.57
                                                                                     L
                                                59.397
                                                         62.421
                             78
                                     141.852
                    LEU
          589
                CD2
 MOTA
                                                                  1.00 28.27
                                                                                     L
                                     140.134
                                                59.314
                                                         66.268
                             78
                     LEU
                C
 MOTA
          590
                                                                  1.00 19.55
                                                                                     L
                                                         67.264
                                                59.809
                                     140.668
                             78
                     LEU
                0
          .591
 MOTA
                                                                  1.00 30.85
                                                                                     L
                                                58.016 65.999
                             79
                                     140.163
                N
                     GLN
          592
 MOTA
                                                                                     L
                                                                  1.00 34.63
                                                         66.859
                                                57.064
                                     140.847
                CA
                     GLN
                             79
           593
 MOTA
                                                                                     L
                                                                  1.00 47.40
                                                         .67.763
                                                56.338
                                     139.855
                             79
                CB
                     GLN
          .594
 MOTA
                                                                                     L
                                                                  1.00 66.32
                                                         68.764
                                                57.238
                                     139.162
                             79
                CG
                     GLN
           595
 MOTA
                                                                  1.00 51.70
                                                                                     L
                                                         69.791
                                                57.793
                                     140.118
                CD
                     GLN
                            .. 79
          .596
 MOTA
                                                                  1.00 38.18
                                                         70.022
                                                                                     L
                                                57.229
                                     141.184
                             79
                OE1
                     GLN
           597 -
 ATOM
                                                                  1.00 50.52
                                                                                     L
                                                58.901
                                                         70.419
                                     139.740
                     GLN
                             79
           598
                NE<sub>2</sub>
 ATOM
                                                                  1.00 36.58
                                                                                     L
                                                         65.965
                                                56:054
                                     141.534
                             79
           599.
                 C
                     GLN
 ATOM .
                                                                                     L
                                                                   1.00 30.40
                                                         64.869
                                                55.755
                                      141.056
                              79
                     GLN
 MOTA
           600
                 0
                                                                                     L
                                                55.504
                                                                   1.00 40.78
                                                         66.430
                                      142.663
                              80
                 N
                     PRO
           601
  MOTA
                                                                                     L
                                                                   1.00 37.68
                                                55.791
                                                         67.740
                                      143.270
                     PRO
                             . 80
 ATOM
                 CD
           602
                                                                   1.00 41.10
                                                         65.665
                                                54.513
                                      143.430
                              80
           603
                 CA
                      PRO
  MOTA
                                                                   1.00 43.39
                                                          66.672
                                                .53.991
                                      144.460
                      PRO
                              80
                 CB
  MOTA
           604
                                                                   1.00 37.64
                                                                                     L
                                                          68.021
                                      144.056
                                                54.557
                     PRO
                              80
                 CG
           605
 ATOM
                                                                   1.00 46.35
                                                                                     L
                                                         65.149
                                                53.398
                                      142.532
                      PRO
                              80
                 C
           606
  ATOM
                                                                                     L
                                                                   1.00 41.86
                                                53.048
                                                          63.969
                                     142.569
                              80
                 0
                      PRO
  MOTA
           607
                                                                                     L
                                                                   1.00 57.27
                                                52.859
                                                          66.056
                                      141.721
                              81
                      GLU
  ATOM
           608
                 N
                                                                                      L
                                                          65.761
                                                                   1.00 58.29
                                      140.793
                                                51.773
                      GLU
                              81
                 CA
  ATOM
           609
                                                                                      L
                                                                   1.00 54.76
                                                          66.967
                                      139.870
                                                51.548
                      GLU
                              81
                 CB
           610
  MOTA
                                                                                      L
                                                                   1.00.71.46
                                                          67.042
                                                 52.498
                              81.
                                      138.677
                 CG
                      GLU
           611
  MOTA
                                                                                      L
                                                                   1.00 74.52
                                                          68.419
                                                 53.125
                                      138.507
                              81
                      GLU
           612
                 CD
  MOTA
                                                                                      L
                                                                   1.00 60.52
                                                          68.983
                                                 53.039
                                      137.390
                              81
                 OEi
                      GLU
           613
  ATOM.
                                                                                      L
                                                                   1.00 65.39
                                                 53.703
                                                          68.934
                                      139.489
                              81
                : OE2
                      GLU
           614
  MOTA
                                                                   1.00 62.35
                                                                                      L
                                                          64.503
                                                 51.998
                                      139.956
                              81
                      GLU
            615
                 C
  MOTA
                                                                   1.00 64.51
                                                                                      L
                                                 51.052
                                                          63.794
                                      139.618
                              81
           616
                 0
                      GLU
  ATOM
                                                                                      L
                                                                   1.00 63.68
                                                 53.256
                                                          64.230
                                      139.629
                              82
                      ASP
  MOTA
            617
                 N
                                                                   1.00 50.22
                                                          63.069
                                                 53.600
                              82
                                      138.823
                      ASP
                 CA
            618
  MOTA
                                                                   1.00 50.14
                                                                                      L
                                                          63.212
                                                 55.024
                                       138.299
                              82
                      ASP
                 CB
            619
  MOTA
                                                                                      L
                                                          64.581
                                                                   1.00 50.17
                                                 55.285
                                       137.729
                              82
                      ASP
            620
                 CG
  MOTA
                                                                   1.00 56.15
                                                                                      L
                                                          65.143
                                      137.107.
                                                 54.358
                              82
                      ASP
                 ODI
            621
  MOTA
                                                                                      L
                                                          65.095
                                                                   1.00 62.15
                                       137.906
                                                 56.408
                 OD2 ASP
                              82
            622.
  MOTA
                                                                                      L
                                                                    1.00 47.40
                                                          61.761
                                                 53.462
                                       139.583
                      ASP
                              82
            623
                  C
  MOTA
                                                                                      L.
                                                                    1.00 44.58
                                                          60.706
                                                 53.837
                                       139.080
                               82
            624
                  0
                      ASP
   MOTA
                                                                                       L
                                                          61.830
                                                                    1.00 43.70
                                                 52.935
                               83
                                       140.801
                      ILE
   MOTA
            625
                  N
                                                                                       L
                                                           60.621
                                                                    1.00 38.44
                                                 52.738
                                       141.586
                               83
                      ILE
                  CA
   ATOM
            626
                                                                                       L
                                                                    1.00 41.83
                                                 52.194
                                                          .60.932
                                       142.991
                               83
                      ILE
            627
                  CB
   ATOM
                                                                    1.00 41.86
                                                                                       L
                                                           59.846
                                                 51,225
                                       143,428
                               83
                      ILE
            628
                  CG2
   MOTA
                                                                                       L
                                                           61.025
                                                                    1.00 52.87
                                                 53.356
                                       143.982
                               83
                      ILE
   MOTA
            629
                  CG1
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				•							•								
ATOM	· 6	30	CD1	ILE		83	٠.	145	.232	53.	032		826			47.1			Ĺ
MOTA	. 6	31	С	ILE	•	83 .	,	140	.827	51.	706		794			32.5			L
MOTA	$\epsilon$	32	0	ILE.		83		140	.588	50.	594	,60 ·	263			26.8			G
ATOM	ε	333	N	ALA		84	•	140	.441	52.	085	58.	. 575	1.	00	26.1	.2	1	Ġ
ATOM	$\epsilon$	534 ·	CA	ALA		84.	. •	139	. 692	51.	200	57	693.			15.1		1	<u>.</u>
, ATOM		335	СВ	ALA		84		. 138	.453	50:	702	58	406	1.	00	21.0	7	. 1	Ļ
ATOM				ALA	٠	84		139	.290	51.	913	56	414	l.	00.	12.9	1	. 1	L
ATOM				ALA	•	84			. 668	53.	060	56	. 195	1.	οó	24.4	4	1	Ŀ
MOTA			N	THR		85		138	.519	51.	224	55	. 578	1.	00	19.6	6	1	<b>L</b> .
ATOM			CA	THR		85		138	.025	51.	774	54	.320	1.	00	17.9	5	3	Ŀ
ATOM			СВ	THR		85			.413	50.	898	53	. 1:31	1.	00	21.8	1	. 1	Ĺ
ATOM			OG1	THR		85			.552	51.	197	52	.024	1.	00	45.1	.2	3	Ĺ
ATOM			CG2	THR		85			.277		435	53	.490	1.	00	27.3	7	. 1	L
			C	THR		85			.505		809		.410	1.	00	27.7	4	. ]	L
MOTA			0	THR		85	•		.876	50.	•	•	.732			32.4			L
ATOM			N	TYR		86		•	.914		960					37.2			L
ATOM	•					86	٠		.469		109		.213			33.3			L
ATOM		546	CA	TYR			•		.153		363		.028			25.3		. ]	
ATOM		547	CB	TYR		86	•		. 852		381		.372			28.5			_ L
ATOM		548	CG	TYR		86					118		.547			44.8			_ L
ATOM		549	CD1			86			.151		071		.789			21.3			L.
ATOM	•		CE1			86			.801 .226		607		.467			14.3			L:
ATOM			CD2	TYR		86.	:		.884		561		,705			22.9		•	L
MOTA		552		TYR		.86		٠.			289		.857			22.2	•		L
MOTA	•	553	CZ	TYR		86			.158		•					25.9			L
MOTA		554	ОН	TYR		86			7.786		210					44.0			L
MOTA	•	655	C	TYR		86	•		.766		159		.868						L
ATOM		656	0	TYR		86			.164				.975			50.7			L
MOTA		657	N	TYR		87			.712		353		.748			51.0			
~ ATOM		658	CA	TYR		87			910		248	•	.526			48.3			L
MOTA	i (	659	CB	TYR		87		• •	795		780		.108			25.2			L
ATOM	i (	<b>660</b>	CG	TYR		87			.108		126		.753			41.4			L T
ATOM	. 1	661		TYR		87	•		.551		080		.427			38.0			L
ATOM	[ (	662	CEl	TYR		87		134	.769		484		.096			42.2			L
ATOM		663	CD2	TYR		87		133	.918	49.	555		.742			33.3			L
ATOM	Ι (	664	CE2	TYR		.87		135	137		957		.418			33.8			L
ATOM	1 . 1	665 ်	CZ	TYR		87		135	.555	.48.	929		. 096			23.9			L
ATOM	E (	666	OH	TYR	•	87		136	5.771	48.	380		.779			34.3			Ŀ
· ATOM	!	667	C	TYR		87	•	130	.493		813		.687			52.:			L
ATOM	[ (	668 ·	0	TYR		87		129	9.948		838		.786			65.			L
ATOM	1	669·	N .	CYS		88		.129	895	53.	250		.582			47.3			L
ATOM	<b>1</b> · •	670	CA	CYS	•	88	•	128	3.538	53.	789		.598			32.			L
ATOM	1	671	C	CYS		88	. <i>'</i>	127	7.715	52.	920	•	.661			32.			L
ATOM	1	672	0	CYS		88			3.140		641	•	.547			39.			L
ATOM	1	673	CB	CYS		88		128	3.530	55.	. 233		.093			33.			Ļ
ATOM	1	674	SG	CYS		88		128	3.799	55.	411		.289			51.			Ļ
ATOM	1	675	N	ĢĿN		89		126	5.549	52.	. 476		.109			22.			L
ATOM		676	CA	GLN		89		125	5.709	51	.648		.260			21.	•		L
ATOM		677	CB	GLN		89		125	5.810	50	. 179	49	.700			.31.			L
ATOM		678	CG	GLN		89		124	1.788	49	.740	50	.735	1	. 00	42.	44		L
ATOM		679	CD	GLN		89	•	·123	3.613	48	982	50	.132			34.			L
ATOM		680		GLN		89		122	2.664	48	. 637	50	.834	1	. 00	26.	74		L
ATOM		681		GLN		89		· 12:	3.671	48	. 723	48	.831	1.	. 00	46.	97.		L
ATOM		682	C	GLN		89		124	1.262	52	.131	49	.287	1	. 00	.25	45		L
	-		_									٠.			•				

	•	•			·		50.313	1.00 20.31	· L
ATOM	`683 ^C	) G	LN	89 .	123.783		48.153	1.00 19.13	L .
MOTA	684	1 G	:LN ·	90	123.574		48.096	1.00 19.46	L
MOTA	685 C	CA G	LN	90 .	122.183			1.00 22.24	. L
MOTA	686	CB G	ELN.	90	121.882		46.769	1.00 22.21	L
MOTA	687 (	cg c	3LN	90	122.072		45.523	1.00 30.31	L.
MOTA	688 (	ם. סב	3LN	90.	120.775	_	45.009	1.00 30.31	L.
ATOM	689	DE1 (	3LN	90 🗒	119.701	51.853	45.586	1.00 32.01	r .
ATOM		NES. (		90	120.878	50.908	43.921	1.00 28.00	· L .
ATOM			<b>3LN</b>	90	121.257		48.267	1.00 30.72	. L
ATOM	692	0 (	<b>3LN</b>	90	121.556 .	50.143	47.801	1.00 25.46	L
ATOM			GLY .	91	. 120.137	51.473	48.951	1.00 34.63	L
ATOM		_	GLY	91	119.166	50.416	49.179	1.00.33.97	. L
MOTA	• -		GLY	91	117.820	50.781	48.580	.1.00 38.48	L
ATOM			GLY	91	116.762	50.335	49.035	1.00 28.43	, L
MOTA			GLN	92.	117.869	51.603	47.540	1.00 28.95	L
ATOM			GLN .	92	116.668 <sup>,</sup>	52.043		1.00 29.94	r r
			GLN	92	116.841	53.489	46.418	1.00 30.37	
MOTA			GLN ·	92	115.571	54.307	46.498	1.00 39.02	L
MOTA			GLN	92	115.079	54.736	45.130	1.00 41.59	· L
ATOM		OE1		92	114.039	54.274	44.663	1.00 31.97	L
MOTA		NE2		92	115.829	55.621	44.479.	1.00 59.08	L
MOTA	703 704	C NEZ.	GLN	.92	116.352	51.144	45.680	1.00 41.66	. L
MOTA		0	GLN	92	115.495	50.267	45.782	1.00 33.85	L.
MOTA	705	N .	THR	93	117.046	51.373	44.564	1.00 60.13	Ĺ
ATOM	706 707 -	CA	THR	. 93 -	116.866	50.596	43.327	1.00 66.93	L
MOTA	•	CB	THR	. 93	117.639	51.242	42.149	1.00 78.05	L
MOTA		OG1		93	117.362	52.647	42.104	1.00 79.52	L
MOTA			THR	93	117.233	50.610	40.829	1.00 75.70	L
MOTA	710		THR	93	117.391	49.180	43.539	1.00.59.06	. L
MOTA	711	C.	THR	93	118.425		44.183	1.00 58.37	r.
MOTA	712	0		. 94	116.703	·	42.993	1.00 50.92	L
MOTA	713	N	TYR	94	117.127		43.209	1.00 52.81	L
MOTA	714	CA.	TYR	94	116.119		42.646	. 1.00 55.69	L
MOTA	715	CB	TYR	94	· i15.809	44.706	43.658	1.00 64.81	L
MOTA	716	CG	TYR	94 ·	116.742		44.643	1.00 66.44	. : <b>L</b>
MOTA	717	CD1		94	116.451		45.622	1.00 61.74	L
MOTA	718	CEI		94	114.573		43.676	1.00 65.08	. L
ATOM	719	CD2	TYR	94	114.269		44.654	1.00 75.90	L,
MOTA	720	CE2		94	115.214		45.623	1.00 73.24	L
MOTA	721	CZ	TÝR	94	114.918		46.603	1.00 71.00	L
MOTA	722	ОН	TYR	94	118.530		42.797	1.00 58.78	L
MOTA	723	C	TYR	94	119.146	-	43.487	1.00 72.46	L
MOTA	72.4	0 .	TYR	95	119.04				; L
ATOM	725	И	PRO	95 .	•				L
ATOM	726	CD	PRO	95	120.41		41.404		·· L
MOTA		CA	PRO		120.67		39.946	1.00 19.42	L
MOTA	728	CB	PRO	95	119.78				L
MOTA	729	CG	PRO	95	121.28				Ļ
MOTA	730	C	PRO	95 95	121.93				L
. ATOM	731	0	PRO	. 96				7 1.00 32.53	L
MOTA	732	N	TYR		122.00	_		8 1.00 29.95	
MOTA	733	CA	TYR	96 96	122.00	-		1 1.00 35.33	. ' <b>r</b>
MOTA	. 734	CB	TYR	. 96	120.83				r
MOTA	735	CG	TYR	96	.20.03				
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. 58
                                                                1.00
                                                                      33
                                                       47.663
                                              45.244
                                   120.678
              CD1
                   TYR
                           96
MOTA
         736
                                                                      23.02
                                                               .1.00
                                                       48.430
                                   119.523
                                              45.087
                           96
         737.
              CEI
                   TYR
ATOM
                                                                1.00 29.21
                                                       46.701
                                             47.244
                                   119.792
                           96
         738
              CD2
                   TYR
MOTA
                                                       47.466
                                                                1.00 29.26
                                              47.096
                                   118.625
                           96
               CE2
                   TYR
         739
MOTA
                                                                1.00 29.92
                                              46.011
                                                       48.329
                                   118.506
                           . 96
               CZ
                   TYR
         740
ATOM
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MOTA
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MOTA
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MOTA
                                                                1.00 36.89
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ATOM
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MOTA
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                                                                                   L
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                                                       41.874
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MOTA
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       . . . 750
MOTA
                                                                                   L
                                                                 1.00 24.58
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MOTA
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MOTA
                                                                                   L
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                    PHE
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MOTA
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                                                                                   L
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                                                                                   L
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 ATOM
                                                                                    L
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                                                                                    L
                                                                 1.00 37.27
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                CA
                                                                                    L
 MOTA
                                                                 1.00 44.52
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          764
 MOTA
                                                                                    L
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                     GLY
 MOTA
          765
                                                                                    L
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                                                        46.008
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                N ·
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 ATOM
                                                                                    Ŀ
                                                        45.848
                                                                 1.00 51.35
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                                     134.600
                           100
                CA
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          767
                                                                                    L
 ATOM
                                                                 1.00 53.12
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                                                                                    L
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 MOTA
                                                                  1.00 26.42
                                                                                    L
                                                         49.504
                                                53.013
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                CA
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                                                                                    Τ.
 MOTA '
                                                                 1.00 21.78
                                                         49.696
                                                54.181
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          .772
                C
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                                                                  1.00 23.28
                                                         48.747
                                                54.886
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                                     136.710
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                0
           773
                                                                                     L
 · ATOM
                                                                1.00 17.65
                                                         50.933
                                                54.392
                                     136.787
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                            102
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                                                                                     L
 MOTA
                                                         51.221 1 00 39.10
                                                55.489
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                            102
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 MOTA
                                                                                     L
                                                                  1.00 49.68
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                                                56.745
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                                                                                     L
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                                                         52.224 1.00 42.53
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                                                                                     L
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                                      139.903
                     LYS
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                                                                                     L
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                                                                   1.00 33.42
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                 CA
                     LYS
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                                                                                     L
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                                                                   1.00 27.82
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                             103
                 CB
                     LYS
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                                                                                     L
 ATOM
                                                         52.937
                                                                   1.00 32.59
                                                54.210
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                                      143.518
                     LYS
           784
                 CG
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                                                                   1.00 39.07
                                                          53.036
                                                55.649
                                      144.038
                             103
                      LYS
           785
                 CD
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                                                                                     L
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                                                          53.790
                                                                        45.98
                                                 55.734
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                      LYS
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                 CE
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                                                          53.258
                                                                   1.00
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                            . 103
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           787
                                                                   1.00
                                                                        23.38
                                                          53.868
                                      141.185
                                                 55.531
                             103
                      LYS
            788
                 C
  ATOM
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					•	·		- 00 30 73	L
MOTA	789	Ο.	LYS	103	140.842	56.687	53.637	1.00 30.72 1.00 32.38	L
ATOM	790	N	LEU	. 104	141.770		55.002		. L
ATOM	791 <sup>.</sup>	CA	·LEU	104	142.077	56.159	56.021	1.00 38.59	· L
ATOM	792 -	CB	LEU .	104	140.904	56.368	56.966	1.00 25.66	Ŀ
ATOM	793	·CG	LEU	104	141.378	57.265	58.113	1.00 32.02	T
ATOM	794	CD1	LEU	.104	140.804	58.658	57.944	1.00 23.79	L
ATOM	795	CD2	LEU	104	140.996	56.648	59.452	1.00 29.54	L
ATOM	796	С	LEU	104 .	143.300	55.784	56.841	1.00 45.89	ŗ.
ATOM	797	0	LEU	104	143.525	54.612	57.154	1.00 45.41	ь Г
ATOM	·798	N	GLU	105	144.080	56.799	57.197	1.00 40.34	P
ATOM	799	CA	GLU	105	145.280	56.597	57.979	1.00 35.75	P
ATOM	800	CB	GLU	105	146.510	56.674	57.064	1.00 52.11	L
ATOM	801	CG	GLU	105	147.798	57.154	57.728	1.00 69.87	. L
ATOM	802	CD	GLU	105	148.876	57.513	56.712	1.00 84.87	L
ATOM	. 803	OEL	GLU	105	150.027	57.054	56.875	1.00 87.68	L.
ATOM	804	OE2		105	148.578	58.251 4		1.00 91.43	L
MOTA	805	C	GLÜ	105	145.365	57.644	59.076	1.00 23.69	L.
ATOM	806	0	GLU	105	145.640		58.808	1.00 36.93	L
ATOM	807	N	ILE	106	145.088	57.241	60.311	1.00 29.41	, L
ATOM	808	CA	ILE	106	145.199	58.168	61.425	1.00 38.27	r L
ATOM	809	CB	ILE	106	144.723	57.513	62.769	1.00 40.94	L
ATOM	810	CG2	ILE	106 ·	145.030	56.026		1.00 31.48	
ATOM	811	CG1		106	145.387	58.193	63.971	1.00 37.37	r L
ATOM	812	CD1	ILE	106	144.571	59.336	64.579	1.00 27.37	•.
MOTA	813	c	ILE	106	146.702	58.441	61.434	1.00 40.57	. L
ATOM	814	· o	ILE	106	147.497	57.506	61.438	1.00 41.72	L
MOTA	815	N	LYS	107	147.088	59.716	61.399	1.00 48.16	, L.
MOTA	816	CA	LYS	107	148.500	60.100	61.364	1.00 42.60	L
MOTA	817	CB	LYS	107	148.640	61.486	60.736	1.00 20.26	r.
MOTA	818	CG	LYS	107	150.043	62.069	60.819	1.00 43.13	L
ATOM	819	CD	LYS	107	150.034	63.572	60.590	1.00 34.99	· L
MOTA	820	CE	LYS	107	149.967	63.895	59.108	1.00 38.89 1.00 13.28	, L
MOTA	821	NZ	LYS	107	148.581	63.791	58.588	1.00 13.28	L
ATOM	822	C	LYS	107	149.186		62.729	1.00 51.05	ŗ
ATOM	823	0	LYS	107	148.643	60.592	63.713	1.00 63.04	ŗ
MOTA	824	N	ARG	108	150.388		62.781	1.00 32.00	L
ATOM	825	CA	ARG	108	151.147		64.028	1.00 33.40	· L
ATOM	826	CB	ARG	108	151.199		64.553	1.00 33.40	Ľ
MOTA	827	CG	ARG	108	152.127		63.771		L
MOTA	828	CD	ARG	108	152.649		64.635		· L
ATOM	829	NE	ARG	108	153.934				· L
ATOM	830	CZ	ARG	108	154.303		66.471		r
ATOM	831	NH	1 ARG	108	153.489		67.224		ŗ
MOTA	832		2 ARG	108	155.484				. L
ATOM	833	C	ARG	108	152.566				L
MOTA	834	0	ARG	108	153.071				· Ľ
ATOM	835		ALA	109			_		r
MOTA	836		ALA	109	154.557				. L
ATOM	837	CB	ALA	109	155.042				Ľ
MOTA	838		ALA	109	155.479				·L
ATOM	. 839	0	ALA	109	155.350				. L
· ATOM	840	N	ASP	110	156403				L
MOTA	841		ASP	. 110	157.350	° 59.784	62.67	. 1.00 03.70	_

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62.082
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                                   158.395
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MOTA
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                                   157.861
                                              61.528
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              CG
ATOM
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                           110
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                                                                                    L
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                    PRO
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                    PRO
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                      ILE
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                                                                                      L
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           889
                                                                   1.00 18.50
                                                          55.632
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                                                                                      L
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                                      169.039
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           891
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                      ILE
                                                                                      L
  MOTA
                                                                   1.00 40.81
                                                          60.076
                                                 39.212
                                      169.467
                             117
                 O
                      ILE
            892
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  MOTA
                                                                    1.00 28.82
                                                 38.560
                                                          58.091
                                      168.626
                             118
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                      PHE
                                                                                      L
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                                                                         22.76
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                                                          58.423
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  ATOM
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L
                                                                1.00 32.60
                                                       58.654
                                    167.260
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                   PHE
                          118
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                                                                1.00 32.33
ATOM
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                          118
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MOTA:
                                                                1.00 32.14
                                                       59.761
                                              38.339
                                    165.845
                          118
               CD1
                   PHE
MOTA
         897
                                                                 1.00 30.97
                                                                                   L
                                                       61.100
                                              36.572
                                    166.731
                          118
                   PHE
               CD2
                                                                                   L
         898
MOTA
                                                                 1.00 43.45
                                                       60.884
                                    165.262
                                              38.902
                           118
               CE1
                   PHE
         899
                                                                                   L
ATOM
                                                                 1.00 24.60
                                                       62.230
                                              37:128
                                    166.148
                           118
                   PHE
         900
               CE2
MOTA
                                                                                   Ľ
                                                                 1.00 41.49
                                                        62.124
                                              38.294
                                    165.411
                           118
                    PHE
               CZ
         901
                                                                                   L
MOTA
                                                                 1.00 26.66
                                                        57.329
                                              36.332
                                    169.339
                           118
                    PHE
               C
ATOM
         902
                                                                 1.00 29.78
                                                                                   L
                                                        56.170
                                              36.370
                                    168.928
                           118
                    PHE
               0
         903
                                                                                   L
MOTA
                                                                 1.00 34.94
                                                        57.685
                                              35.602
                                    170.402
                           119
               Ν.
                    PRO
         904
                                                                                    L
MOTA
                                                                 1.00 32.83
                                                        59.027
                                              35.559
                                    170.999
                           ,119
                    PRO
         905
               CD
                                                                                    L
MOTA
                                                                 1.00 37.60
                                                        56.734
                                              34.763
                                    171.136
                           119
                    PRO
         906
               CA
                                                                                    L
MOTA
                                                                 1.00 31.28
                                               34.369
                                                        57.497
                                    172.400
                           119
                    PRO
         907
               CB
                                                                                    L
MOTA
                                                                 1.00
                                                                       32.18
                                                        58.732
                                               35.261
                                    172.428
                           119
               CG
         908
                    PRO
                                                                                    L
ATOM
                                                                 1.00
                                                                       36.29
                                                       56.389
                                               33.551
                                    170.278
                           119
                C
                    PRO
          909
                                                                                    L
MOTA
                                                                 1.00
                                                                       43.06
                                               33.266 - 57.079
                                    169.297
                           119
                    PRO
          910
               0
                                                                 1.00 33.16
MOTA
                                                        55.321
                                               32.822
                                    170.628
                    PRO
                           120
          911
               N
ATOM
                                                                 1.00 35.66
                                                        54.401
                                    171.752
                                               33.046
                           120
                    PRO
                CD
          912
                                                                                    L
 MOTA
                                                                 1.00 27.25
                                                        54.944
                                    169.838
                                               31.645
                           120
                    PRO
                ·CA
          913
                                                                                    L
 ATOM
                                                                 1.00 23.84
                                                        53.699
                                    170.543
                                               31.110
                     PRO
                            120
                CB
          914
                                                                                    L
 ATOM
                                                                 1.00 47.85
                                                       . 53.186
                                               32.258
                                     171.345
                     PRO
                            120
                CG
 MOTA
          915
                                                                  1.00 47.51
                                                                                    L
                                               30.597
                                                        56.052
                                     169.771
                     PRO
                            120
          916
                C
                                                                                     T.
 MOTA
                                                                  1.00
                                                                       61.24
                                                        57.097
                                               30.733
                                     170.408
                            120
          917
                0
                     PRO
                                                                                     L
 MOTA
                                                                 1.00 46.49
                                               29.552
                                                         55.812
                                     168.990
                            121
                N
                     SER
          918
                                                                                     L
 MOTA
                                                                  1.00 35.79
                                                         56.781
                                               28.481
                                     168.836
                            121
                CA
                     SER
          919
                                                                                    L
 MOTA
                                                                  1.00 39.97
                                              .28.091
                                                        .56.908
                                     167.366
                            121
                CB
                     SER
          920
                                                                                     L
 ATOM
                                                                  1.00
                                                                       61.95
                                                         58.153
                                     166.848
                                               28.512
                            121
                OG
                     SER
          921
                                                                                     L
 MOTA
                                                                  1.00
                                                                       35.14
                                                         56:366
                                               27.264
                                     169.643
                            121
          922
                C
                     SER
                                                                                     L
 ATOM.
                                                                  1.00 54.90
                                                         55.178
                                                26.970
                                     169.776
                            121
                     SER
                0
          923
                                                                                     L
                                                                  1.00 34.00
 MOTA
                                                26.566
                                                         57.352
                                     170.190
                            122
                     SER
                N
                                                                                     L
           924
 MOTA
                                                                  1.00
                                                                       43.67
                                                         57.078
                                                25.367
                                     170.964
                            122
           925
                CA
                     SER
                                                                                     L
MOTA
                                                                  1.00
                                                                       55.34
                                                         58.385
                                                24.661
                                     171.319
                            122
           926
                CB
                     SER
                                                                                     L
                                                                        66.58
 MOTA
                                                         59.496
                                                                  1.00
                                     170.845
                                                25.401
                            122
                     SER
           927
                OG
                                                                                     Ĭ
 MOTA
                                                                        39.48
                                                                  1.00
                                                         56.265
                                     170.038
                                                24.496
                            122
                     SER
                 C
 ATOM
           92B
                                                                        38.43
                                                                                     L
                                                                  1.00
                                                         55.139
                                                24.107
                                      170.345
                     SER
                            122
                 O
           929
                                                                                     L
 MOTA
                                                                  1.00
                                                                        39.62
                                                         56.850
                                      168.878
                                                24.223
                            123
                     GLU
                N.
           930
                                                                                     L
  ATOM
                                                                        42.31
                                                         56.208
                                                                   1:00
                                                23.412
                                      167.865
                     GLU
                            123
                 CA
           931
                                                                                     L
                                                                   1.00 49.13
  ATOM
                                                23.487
                                                         57.012
                                      166.569
                     GLU
                            123
                 CB
           932
                                                                                     L
  ATOM
                                                                   1.00 85.24
                                                          56.294
                                                22.895
                                      165.364
                            123
           933
                 ÇG
                     GLU
                                                                                     L
                                                                   1.00100.00
  MOTA
                                                22.520
                                                          57.240
                                      164.237
                             123
           934
                 CD
                     GLU
                                                                                     L
                                                                   1.00 99.99
  MOTA
                                                          58.473
                                                22.525
                                      164,458
                             123
                 OE1 GLU
           935
                                                                                      L
                                                                   1.00 99.98
  MOTA
                                                          56.742
                                      163.127
                                                22,221
                 OE2 GLU
                             123
                                                                                      L
           936
                                                                   1.00 34.58
  MOTA
                                                         .54.774
                                      167.627
                                                23.885
                     GLU
                             123
                                                                                      L
           937
                 С
  MOTA
                                                                   1,00 33.93
                                                          53.843
                                                23.079
                                      167.599
                             123
                      GLU
           938
                 0
                                                                                      L
                                                                   1.00 36.30
  MOTA
                                                          54.588
                                                25.193
                                      167.467
                             124
                      GLN
                 N
           939
                                                                   1.00 21.55
                                                                                      L
  ATOM
                                                 25.719
                                                          53.254
                                      167.228
                      GLN
                             12,4
            940
                 CA
                                                                                      L
 ATOM
                                                                   1.00 32.12
                                                          53.289
                                      166.875
                                                 27.207
                             124
            941
                 CB
                      GLN
                                                                   1.00 35.77
                                                                                      L
  ATOM
                                                 27.854
                                                          51.927
                                      167.075
                             124
            942
                 CG
                      GLN
                                                                                      L
                                                                   1.00 35.92
  ATOM
                                                         .51.766
                                                 29.160
                                       166.351
                             124
                      GLN
            943
                 CD
                                                                   1.00 37.01
                                                                                      L
  ATOM
                                                          52.669
                                                 29.995
                                       166.349
                             124
                      GLN
            944
                 OE1
                                                                                      L
  MOTA
                                                                   1.00 40.10
                                                          50.603
                                       165.739
                                                 29.355
                             124
                 NE2
                      GLN
                                                                                      Ľ
            945
                                                                   1.00 29.80
  ATOM
                                                          52,353
                                                 25.534
                                       168.441
                             124
                  C
                      ·GLN
                                                                                      L
            946
                                                                   1.00 40.34
   ATOM
                                                 25.269
                                                          51.159
                                       168.308
                             124
                      GLN
            947
                  0
   MOTA
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			•					1.00 29.81	L ·
ATOM	948	N	LEU	125	169.626		52.921 52.142	1.00 29.61	L
MOTA	949	CA	LEU	125	170.837			1.00 28.95	L
ATOM	950	CB	LEU	125	172.047		52.998	1.00 28.05	. L
ATOM	951	CG	LEU	125 :	172.296	27.418	53.004	1.00 35.58	. L
ATOM	952	CD1	LEU	125		27.794		1.00 18.04	L
ATOM	953	·CD2	LEU	125	172.814		51.636	1.00 31.63	L.
ATOM	954	С	LEU	125	170.952	24.108	51.630	1.00 31.03	L
ATOM	955	0	LEU	125	171.396	23.873	50.503	1.00 28.04	Li
ATOM	956	N	THR	.126	170.530	23.156	52.454	1.00 34.33	L
ATOM	957	CA	THR	126	170.570	21.741	52.094	1.00 47.29	Ľ.
ATOM	958	CB	THR	126	169.981	20.876	53.226	1.00 47.25	L
ATOM	959	OG1	THR	126	170.445	21.364		1.00 58.05	· L
ATOM	960	CG2		126	170.397	19.426	53.063	1.00 47.30	L
ATOM	961	C	THR	126	169.806	21.444	50.796		L
ATOM	962	.0	THR	126	170.142	20.515	50.063	1.00 54.95	L
•	963	N	SER	127	168.779	22.236	50.513	1.00 57.73	L
ATOM ATOM	964	CA	SER	· 127	167.985	22.042	49.308	1.00 63.60	L
	965	CB	SER	12.7	166.551	22.525	49.542	1.00 63.78	L
MOTA	966	OG	SER	127	166.528	23.787	50.186	1.00 64.66	· L
MOTA	967	C	SER	127	168.581	22.760	48.096	1.00 67.39	P.
ATOM	968	, 0	SER	127	168.031	22.693	46.994	1.00 73.65	L
MOTA	969	N	GLY	128	169.701	23.446	48.303	1.00 60 63	L
ATOM	970	CA	GLY	128	170.350	24.154	47.209	1.00 50.24	L
MOTA	971	C	GLY	128	169.838	25.563	46.947	1.00 51.09	. Ţ
MOTA	972	0	·GLY	128	170.151	26.169	45.917	1.00 49.56	r L
ATOM	973	N	GLY	.129	. 169.043	26.083	47.877	1.00 48.06	. <b>L</b>
ATOM	974	· CA	GLY	129	168.507	27.425	47.731	1.00 48.39	. L
MOTA		·C	GLY	129	168.926	28.261	48.919	1.00 45.57	. L
ATOM	975		GLY	129	169.221	27.719		1.00 58.83	· L
MOTA	976		ALA	130	168.964	29.577	48.746	1.00 44.51	· · L
MOTA	977 978			130	169.368	30.467		1.00 42.67	. L
ATOM	979			130	170.868		49.766		L L
ATOM	980		ALA	130	168.612	31.784	49.784		· L
ATOM	981		ALA	130	168.661	32.506	48.783		. L
MOTA	982		SER	131	167.923				Ľ
MOTA	983			131	167.154	33.334	50.936		L
ATOM	984			131	165.662		51.035		L
MOTA	985			131	165.165	32.494			L.
MOTA	986		SER	131	167.568				·L
MOTA	987		SER	131	167.547	33.714			L
MOTA MOTA	988		VAL	132	167.958	35.413			. T
	989			132	168.353				L
ATOM . ATOM	99			132	169.558				L
	99		31 VAL	132	170.32		_		L
MOTA .	99		32 VAL	132	.170.46	B 36.420			P.
	99		VAL	132	167.14				L
ATOM	. 99	_	VAL	132	166.60		_		L
ATOM	99			133	166.70	1 37.314			L
MOTA	99	_		133	165.53	2 (38.10			L
MOTA	99				164.48	3 37.23			L
MOTA			G1 VAL		163.38	2 38.11			
MOTA	. 99 99		G2 VAL		163.90	0 36.21	1 54.46		. <u>.</u>
ATOM	100				165.87	0 39.29	6 55.54	8 1.00 10.26	
MOTA	100	-						•	

							20 202	56.454	1.00 2	24.39	- 1	Ţ.
MOTA	1001 .	0 7	<b>VAL</b>	133		5.701	39.222	55.254	1.00 2			Ŀ
MOTA	1002	И	CYS.	134	•	5.206	40.404 41.626	55.999	1.00			. نڌ
MOTA	1003	CA	CYS	134		5.412		56.444	1.00			L
MOTA	1004	Ċ (	CYS	134		4.070	42.163		1.00			L
ATOM	1005	0	CYS	134		3.166	42.338	55.631	1.00			L
ATOM	1006	CB	CYS	134		6.104	42.660	55.127	1.00		•	L
MOTA	1007	SG	CYS	134		6.705	44.083	56.077	1.00			L
ATOM	1008	И.	PHE	135	16	3.946	42.420	57.737	1.00			L
ATOM	1009	CA	PHE	135		2.710	42.949	58.296	1.00		•	L
ATOM	1010		PHE	135		2.297		59.536				L
ATOM	1011		PHE	135		1.854	40.746	59.244	1.00	58.79		L.
ATOM	1012	CD1	PHE	135	16	0.991		58.187			٠.	L.
ATOM-	10:13		PHE	135		2.280	39.696	60.049		38.90		L .
ATOM ·	1014	CE1		135	16	0.555	39.170			56.32	•	L
ATOM	1015	CE2	PHE	135	16	1.849	38.391	59.810		57.18		L
	1016	CZ	PHE	135 .	16	0.987		58.753		46.88		L
ATOM	1017	C	PHE	135	1,6	2.880	44.412			37.21	•	L
MOTA	1017	0	PHE	135	1.6	3,841	44.773	59.373		31.75	•	
MOTA	1019	N.	LEU	136	. 16	51,951	45.253	58.264		38.27		L
ATOM		CA.	LEU	136	16	51,968	46.665			33.10	•	r
ATOM	1020	CB	LEU	136		52.049	47.531	57.369		23.62		L
MOTA	1021		LEU	136	16	53.303	47.259	56.534		17.58		L
MOTA	1022	CG	LEU	136		63.055	46.103	55.572		17.79		L
MOTA	1023	CDI	LEU	136		63.686				29.81		L
MOTA	1024			136		60.632		59.319		30.65		L
MOTA	1025	·C	LEU	136		59.600		58.673		30.43		L
ATOM	1026	<u>o</u> .	LEU	137		60.651				35.92		L
MOTA	1027	N	ASN	137		59.421				43.25	•	L
MOTA	1028	CA	ASN	137		59.387				42.56		L.
MOTA	1029	CB	ASN	137		59.308	•			30,61		L
MOTA	1030	CG				59.471			1.00	37.72		L.
ATOM	1031		ASN	137	•	59.057		_		39.03		L
MOTA	1032	ND2		137		59.101			1.00	40.01		L
MOTA	1033	C	ASŅ	137 137		59.975				39.51		L.
MOTA	1034	0	asn			57.813			1.00	41.07		L
ATOM	1035	N	ASN	138			49.526		1.00	38.43		L
MOTA	1036	CA.		138		.57.227				34.91		L
MOTA	1037	CB	ASN	138		56.667			1.00	33.75		L
MOTA	1038	CG	ASN	138		155.592				29.26		L
MOTA	1039		ASN	138		L57.402		4 . 64 . 537		33.12		L
MOTA		_	ASN	138		L57.23.				31.73		Ŀ
MOTA	1041		ASN	138		158.58	-	7 63.55		39.37		L
MOTA	1042		ASN	.138		157.49			9 1.00	32.60		L
MOTA	1043		PHE	139		157.98				34.36		L
MOTA	1044		PHE	. 139		159.13				37.95		L
MOTA	1045		PHE	139		158.77				21.99		L
MOTA	1046	CG	PHE	139						0 28.23	•	L
MOTA	∵1047		1 PHE	139		158.29				0.23.34		L
MOTA	1048		2 PHE	139		158.94				0 22:39		·L
MOTA	. 1049	CE	1 PHE	139		157.99	_			0 15.56		L
ATOM	1050			139		158.64				0 21.70		L
MOTA	1051	L CZ		139		158.17				0 42.27		L
MOTA		2 C	PHE	139		156.86		2 60.35		0 50.50		L
MOTA		3 0	PHE	. 139		155.77	2 53.14	2, 60.35				
					•			•		•		•

	•					54.906 ·	60.444	1.00 53.69	L
MOTA	1054	N	TYR	140		55.847	59.883	1.00 47.40	L
MOTA	1055	CA	TYR	140			60.942	1.00 53.56	L
MOTA	1056	CB .	TYR	140 .		56.266	60.360	1.00 71.75	r
ATOM	1057	CG	TYR	140	154.002	_		1.00 76.99	L
MOTA	1058	CD1	TYR	140	154.072		60.029	1.00 91.66	r.
ATOM	1059	CE1	TYR	140	152.978	58.991	59.471	1.00 91.00	L.
ATOM .	1060	CD2	TYR	140	152.809	56.301	60.119		L
MOTA	1061	CE2	TYR	140	151.712	56.948	59.562	1.00 96.08	L
	1062	CZ	TYR	140	151.803	58.293	59.242	1.00 93.77	· L
MOTA	1063	OH	TYR	140	150.716	58.946	58.706	1.00 99.99	r.
ATOM	1064	C	TYR	140	156.981	57.065	59.410	1.00 31.82	L
MOTA	1065	0	TYR	140	157.900	57.515	60.088	1.00 34.79	L
MOTA		N	PRO	141 .	156.631	57.613	58.240	1.00 33.26	
MOTA	1066		PRO	141	157.366	58.764	57.691	1.00 26.57	L ·
MOTA	1067	CD	PRO	141	155.566	57.178	57.336	1.00 39.66	L
MOTA	1068	CA.		141	155.450	58.321	<b>56.323</b>	1.00 45.22	L
MOTA	1069	CB	PRO		156.359	59.402	56.804	1.00 34.28	<b>r</b>
MOTA	1070	CG	PRO	141	155.882	55.860	56.651	1.00 32.49	L
MOTA	. 1071	C,	PRO	141	156.913		.56.913	1.00 34.82	L
MOTA	.1072	Ο.	PRO	141	154.986	55.438	55.762	1.00 33.41	: L
ATOM	1073	И	LYS	142	155.157	54.191	55.033	1.00 45.13	· L
MOTA	1074	CA	LYS	142	153.862	53.816	54.304	1.00 63.72	L,
ATOM .	1075	CB	LYS	142		54.942	54.200	1.00 82.02	$\cdot$ ${f L}$
. ATOM	1076	CG	LYS	142	152.851	54.806		1.00 86.08	Ľ
MOTA	1077	CD	LYS	142	152.005		52.114	1.00 97.81	L .
ATOM	1078	CE	LYS	142	152.031		51.209		L
MOTA	1079	NZ	LYS .	142	153.221	56.173	54.029		L
MOTA	. 1080	C	LYS	142	156.290	54.308	53.679		· L
ATOM	. 1081	0	LYS	142	156.926	53.320			L
MOTA	1082	N	ASP	143	156.543	55.523	52.603		L
ATOM	1083	CA	ASP	143	157.605	55.725	52.259		L
ATOM	1084	CB	ASP	143	157.730		51.286		.L
ATOM	1085	· CG	ASP	143	156.674	57.656			L
ATOM	1086		L ASP	143	155.526	57.891			· <b>L</b>
ATOM	1087	OD:	2 ASP	143	156.992				L
ATOM.	1088	C	ASP	143	158.923				L
ATOM	1089		ASP	143	159.344				L
ATOM	1090		ILE	144	159.563	54.348			L
	1091			. 144	160.839			1.00 51.41	L
MOTA	1092			144	160.664				L
MOTA MOTA				144	160.074	51.392			
	1094			144	162.011				r L
MOTA	1095	•		144	161.892	51.470	55.67		
MOTA	1096		ILE	144	161.441	L 53.160	51.46	0 1.00 48.41	
MOTA			ILE	144	160.719	52.739			
MOTA	1097	•	ASN	145		53.142			L
ATOM	1098			145	163.447		50.22	1 1.00 62.49	
ATOM	1099			145	164.063		49.39	9 1.00 75.48	L
MOTA	1100			145	164.104	4 53.413	3 47.92	2 1.00 98.08	
MOTA	1101		) ASN	145	163.684		1 47.09	4 1.00 99.97	
· ATOM	110				164.61			9 1.00 99.99	L
MOTA	110	_	2 ASN	. 145	164.53	_		0 1.00 52.75	
ATOM.	1104		ASN		165.53			1 1.00 46.53	
ATOM			ASN		164.32		2 50.33		5 L
MOTA	110	6 N	VAL	146	104.32	- =	•	•	•

•		_				165.283	49.327	50.683	1.00 55.40		L
MOTA	1107	ĊA	VAL	146		164.572	48.048	51.171	1.00 51.60		Ľ
MOTA	1108	CB	VAL	146		165.593	47.066	51.728	1.00 23.45		L
MOTA	1109	CG1		146			48.397	52.234	1.00 57.40	•	L
ATOM	1110	CG2		146		163.545	48.975	49.490	1.00 53.23		L.
MOTA	1111	C	VAL '	146		166.158	48.977	48.341	1.00 69.79	٠.	Ļ
ATOM	1112	Ο.	VAL ·	146		165.707		49.775	1.00 49.86	٠.	L
MOTA	1113	N	LYS	147	•	167.421	48.679	48.746	1.00 42.42		ъ.
MOTA	1114	ĊA	LYS	147		168.378	48.312	48.413	1.00 47.62		r.
MOTA	1115	CB	LYS	147	<i>:</i>	169.281		47.302	1.00 79.82		L
MOTA	1116	CG	LYS	147		168.754	50.388	46.512	1.00 86.84		L
MOTA	1117	CD	LYS	147		169.895	51.010		1.00.93.63		L
MOTA	1118	CE	LYS	147		169.939	52.524	46.691	1.00.75.73	•	r.
MOTA	1119	NZ	LYS	147		170.983	52.943	47.671	1.00 75.75	•	L
ATOM	1120	C	LYS	. 147		,169.222 <sub></sub>	47.159	49.265	1.00 33.30		L
ATOM	1121	o i	LYS	147	•	169.545	47.103		1.00 22.60		L
ATOM	1122	N	TRP	148		169.566	46.236	48.375			L
ATOM	1123	CA	TRP	148	•	170.386		48.758	1.00 34.06	•	L
ATOM	1124	CB	TRP	148	٠	169.782	43.796	48.214	1.00 32.94		L
ATOM	1125	CG.	TRP	.148		168.782	43.185	49.150	1.00 47.82		L
ATOM	1126	CD2	TRP	148		169.062	42.433	50.338	1.00 46 07		L
ATOM	1127			148		167.822	42.096	50.923	1.00 40.42		L
MOTA	1128	CE3		148		170.243	42.012	50.967	1.00 64.21		. P
ATOM .		CD1		148		167.420	43.270	49.065			. Г
ATOM	1130		TRP	148		166.838	42.621	50.125	1.00 38.06	·	
ATOM	1131		TRP	148		167.725	41.357	52.109	1.00 15.75		L
ATOM	1132	CZ3		.148.		170.146	41.277	52.148	1.00 72.60		L
MOTA	1133	CH2		148		168.894	40.958	52.705	1.00 49.76		L
ATOM	1134	C	TRP	148		171.793	45.269	48.217	1.00 36.36	•	L L
ATOM	1135	ō	TRP	148		171.984	45.624	47.055	1.00 34.43		
ATOM	1136	N	LYS	149	•	172.784	45.027	49.062	1.00 44.04		L
ATOM	1137	CA	LYS	149		174.157	45.161	48.623			r L
MOTA	1138	CB	LYS	149		174.820	46.341	49.321			L
	1139	CG	LYS	149		175.080	47,.515	48.400			L
ATOM ATOM	.1140	CD	LYS	149		174.417		48.915			L
MOTA	1141		LYS	149	•	175.294	49.986	48.667			. ţ
MOTA		·NZ	LYS			175.270	50.930				L
MOTA ·	1143	C	LYS		٠	174.937	43.893		1.00 38.62		L L
ATOM	1144	ō	LYS	149		175.125	43.505				. <b>.</b>
ATOM	1145	N	ILE	150		175.372					L
ATOM	1146		•	150 `		176.157					L
ATOM	1147			150		175.675	40.954		41		L
ATOM	1148			150		176.371				•	P.
ATOM	1149			150		174.159	40.812				L
MOTA	. 1150		1 ILE	150		173.598				•	L
ATOM	1151		ILE	150		177.600	42.361				L
	1152	_	ILE	150		177.975	42.479				
MOTA	1153		ASP	151		178.404					L.
ATOM	1154			151		179.805	42.886				L
MOTA	1155			151		180.507	41.896		1.00 74.75	٠.	
ATOM	1156			151	·	180.844					L
MOTA	1157		1 ASP			180.681					· L
MOTA	1158		2 ASP			181.274		•			L
MOTA	1159				•	179.854		47.90	5 1.00 70.87		L
atom	TTO		·				•				

		٠.			180.483	44.536	46.868	1.00 70.42	· L
MOTA	1160	0	ASP	151	179.172		48.577	1.00 76.86	· r
MOTA	1161	N	GLY	152 .	179.172	46.613	48.139	1.00 67.78	, L
MOTA	1162	CA	GLY.	152	178.418	46.840	46.824	1.00 70.46	. L
MOTA	1163	· C	GLY	152		47.980	46.438	1.00 79.32	L
MOTA	1164	0	GLY	152	178.156	45.754	46.131	1.00 62.96	L
MOTA	1165	N	SER	153	178.098	45.845	44.856	1.00 60.58	L
MOTA	1166	CA	SER	153	177.409	44.693	43.947	1.00 68.60	L
MOTA	1167	CB	SER	1.53	177.840		42.653	1.00 71.40	, L
MOTA	1168	OG	SER	153	178.171	45.160	45.063	1.00 61.38	L
ATOM	1169	С	SER	153	175.902	45.800	45.895	1.00 59.28	L
MOTA	1170	0	SER	153	175.401	45.044	44.304	1.00 59.43	L.
MOTA	1171	N	GLU	154	175.183	46.620		1.00 66.09	L
ATOM	1172	CA	GLU	154 ·	173.731	46.677	44.393	1.00 81.88	L
MOTA	1173	CB	GLU	154	173.222	47.987	43.793	1.00 78.09	L
ATOM	1174	CG	GLU	154	172.299	48.776	44.700	1.00 85.76	L
MOTA	1175	CD	GLU	154	171.857	50.087		1.00 65.69	L
MOTA	1176	OE1	GLU	154	170.891	50.074	43.283	1.00 98.75	r
MOTA	1177	OE2		154	172.476	51.131	44.385		L
ATOM	1178	С	GĻU.	154	173.123	45.505	43.635	1.00 78.80	· L
MOTA	1179	0	GLU	154	173.476	45.248		1.00 87.43	L
ATOM .	1180	N	ARG	155	172.211			1.00 78.61	· L
ATOM	1181	CA	ARG	155	171.552	43.654	43.669	1.00 72.18	L
ATOM	1182	CB	ARG	155	171.904	42.371	44.411	1.00 57.25	L
MOTA	1183	CG	ARG	155 ·	172.051	41.177	43.500	1.00 53.97	L
ATOM	1184	CD	ARG	.155	170.868	40.250	43.648	1.00 47.95	. L
ATOM	1185	NE	ARG	155	170.680	39.401	42.474	1.00 59.26	. L
	1186	CZ	ARG	155	171.533	38.459	42.084	1.00 47.18	
ATOM'	1187		L ARG	155	172.644	38.239	.42.776	1.00 58.65	. L
MOTA	1188		2 ARG	155	.171.272	37.731	41.007	1.00 62.18	L
ATOM	1189	C	ARG	155	170.049	43.862	43.692	1.00 76.06	L
MOTA	1190	o	ARG	155	169.470	44.142	44.741	1.00 79.59	L
MOTA.	1191		GLN	156	169.426	43.726	42.527	1.00 81.46	L
ATOM	1192	CA			167.984	43.913	42.395	1.00 75.51	. L
MOTA	1192			156	167.702	45.122	41.510	1.00 76.21	. L
MOTA				156	168.779		41.579	1.00 86.59	L
MOTA	. 1194			156	168.216				T
ATOM	1195			156	167.460		40.597	1.00 74 92	L
MOTA	1196		•	156	168.579		42.486	1.00 79.96	L
MOTA.	1197	_	GLN	156	167.308	42.690	41.799	1.00 75.18	L
ATOM.	1198 1199		GLN	156	166.094	42.663			L
MOTA.	1200		ASN	157	168.106	41.681	41.485	1.00 69.92	L
MOTA	1200			157	167.577		40.909	1.00 62.62	, Ī
ATOM	1201			157	168.587	39.880	39.912	1.00 83.40	L
ATOM			ASN	157	168.058		39.189	1.00 96.73	. L
MOTA	1203	•	1 ASN	157	168.142		39.692		L
MOTA	1204		2 ASN	157	167.509		38.000		L
MOTA	1205			157	167.270		42.009	1.00 43.07	L
ATOM	. 1206		ASN	157	168.169	38.978			L
MOTA	1207		GLY	158	165.99			5 1.00 37.93	L
MOTA	1208			•	165.613			3 1.00 45.50	r
MOTA	1209	_			165.05			1 1.00 46.88	· r
MOTA	1210	_			164.90			8 1.00 46.67	
MOTA	121				164.73	_	5 44.40	9 1.00 46.40	, L
MOTA	121	2 N	VAL					•	

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L
                                                               1.00 48.04
                                                      45.582
                                   164.191
                                             40.668
                          159
              CA
                  . VAL
       1213
MOTA
                                                                                  ·L
                                                      45.707
                                                               1,00 46.84
                                   164.746
                                             42.089
                   VAL
                          159
              CB
        1214
ATOM
                                                                                  L
                                                      .47.106
                                                               1.00 49.41
                                             42.616
                                   164.497
                          159
                   VAL
              CG1
ATOM
        1215
                                                                                  L
                                                               1.00 31.32
                                                      45.398
                                             42.091
                                   166.234
              CG2
                          159
                   VAL
        1216
MOTA
                                                                                  L
                                                                1.00 50.14
                                             40.738
                                                      45.570
                                   162.668
                   VAL
                          159
              С
        1217
                                                                                  L
MOTA
                                                                1.00 70.43
                                                     44.563
                                   162.065
                                             41.111
                          159
              O
                   VAL
        1218
                                                                                  ·L
MOTA
                                                                1.00 47.07
                                                       46.699
                                             40.371
                                   162.060
                          160
                   LEU
        1219
              N
ATOM
                                                                                  L
                                                                1.00 40.66
                                                       46.862
                                   160.606
                                             40.379
                          160
                   LEU
        1220
               ÇA
MOTA
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                                                                1.00 28.04
                                                       46.894
                                             38.958
                                   160.060
                          160
               CB
                   LEU
MOTA
        1221
                                                                                  L
                                                                1.00 32.43
                                                       45.577
                                              38.197
                                   160.148
                   .LEU
                          160
        1222
               CG
                                                                                  L
MOTA
                                                                1.00 37.34
                                                      45.669
                                   159.270
                                              36.965
                          160
        1223
               CD1 LEU
                                                                                  L
MOTA
                                                                1.00 7.94
                                                       44.413
                                              39.095
                                    159.722
                          160
               CD2 LEU
        1224
MOTA
                                                                1.00 42.42
                                                       48.151
                                              41.077
                                    160.204
                           160
                    LEU
        1225
               C
MOTA
                                                                                  L
                                                                1.00.48.94
                                              40.583
                                                       49.250
                                    160.474
                           160
        1226
               0
                    LEU
MOTA
                                                                1.00 40.58
                                                                                  ۲.
                                              42.220
                                                       48.011
                                    159.545
                          161
               N
                    ASN
        1227
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MOTA
                                                                1.00 26.69
                                                       49.161
                                              42.996
                                    159.109
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                    asn
        122B
               CA
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MOTA
                                                                1.00 24.90
                                                       48.917
                                              44.477
                                    159.377
                           161
                    ASN
        1:229
               .CB
 ATOM
                                                                1.00 36.23
                                                       48.500
                                              44.746
                                    160.804
                           161
                  · ASN
        1230
               ÇG
MOTA
                                                                1.00 55.57
                                                       49.153
                                              44.301
                                    161.743
                           161
               OD1 ASN
         1231
                                                                                   L
 MOTA
                                                                 1.00 47.35
                                                       47.407
                                              45.475
                                    160.975
                           161
               ND2 ASN
         1232
                                                                                   L
 MOTA
                                                       49.471
                                                                .1.00 32.25
                                              42.792
                                    157.637
                           161
                    ASN
               C
         1233
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                                                                 1.00 34.73
 MOTA
                                                        48.605
                                              42.415
                                    156.850
                           161
                    ASN
         1234
               0
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 MOTA
                                                                 1.00 28.82
                                                        50.722
                                               43.052
                                    157.276
                    SER
                          .162
               N
         1235
                                                                                   L
 MOTA
                                                                 1.00 30.10
                                              42.907
                                                        51.179
                                    155.908
                           162
                CA
                    SER
        .1236
                                                                                   L
 MOTA
                                                                 1.00 25.07
                                              41.470 . 51.623
                                    155.655
                           162
                CB
                    SER
         1237
                                                                                   L
 MOTA
                                                                 1.00 34.98
                                              41.341
                                                        52.203
                                    154.368
                           162
                    SER
                OG
 ATOM
         1238
                                                                 1.00 28.22
                                                                                   L
                                               43.855
                                                        52.349
                                    155.687
                    SER
                           162
                C
         1239
                                                                 1.00 28.01
                                                                                   L
 ATOM
                                               43.949
                                                        53:231
                                     156.542
                           162
                0
                    SER
         1240
                                                                 1.00 44.68
                                                                                   L
 ATOM
                                                        52.346
                                               44.560
                                     154.556
                            163
                    TRP
         1241
                N
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                                                                                    L
 ATOM
                                                        53.413
                                               45.502
                                     154.217
                            163
                     TRP
                CA
         1242
                                                                 1.00 47.04
                                                                                    L
 MOTA
                                               46.914
                                                        52.865
                                     153.977
                     TRP
                            163
         1243
                CB
                                                                                    L
 MOTA
                                                                 1.00 50.28
                                                        52.139
                                               47.542
                                     155.114
                CG
                     TRP
                            163
         1244
                                                                                    L
                                                                 1.00 47.77
 MOTA
                                                        50.824
                                               47.209.
                                     155.581
                            163
         1245
                CD2
                     TRP
                                                                                    L
                                                                 1.00 47.30
 MOTA
                                                        50.529
                                   156.655
                                               48.079
                            163
                     TRP
         1246
                CE2
                                                                                    L
 ATOM
                                                                 1.00 36.64
                                                        49.865
                                               46.258
                                     155.193
                            163
                     TRP
                CE3
         1247
                                                                                    L
 ATOM
                                                                 1.00 61.33
                                                        52.578
                                     155.899
                                               48.573
                            163
                CD1 TRP
         1248
                                                                                    L
 MOTA
                                                                  1.00 51.73
                                                        51.615
                                               48.901
                                    156.828
                            163
                     TRP
                NĘ1
          1249
                                                                                    L
  MOTA
                                                                 1.00 41.27
                                                         49.313
                                                48.028
                                     157.349
                            163
                CZ2
                     TRP
          1250
                                                                                    L
  MOTA
                                                                  1.00 43.64
                                                         48.655
                                               46.206
                                     155.882
                CZ3
                     TRP
                            163
          1251
  ATOM
                                                                  1.00 31.42
                                                                                    L
                                                        48.391
                                                47.089.
                                     156.950
          1252
                 CH2
                     TRP
                            163
  ATOM
                                                                                    L
                                                                  1.00 47.66
                                                         54.111
                                                45.087
                                     152:937
                            163
          1253
                C
                     TRP
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  ATOM
                                                                  1.00 46.95
                                                        53.504
                                                44.487
                                      152.056
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                     TRP
          1254
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  MOTA .
                                                                  1.00 42.09
                                                45.420 55.389
                                     152.831
                     THR
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                 N
          1255
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  MOTA
                                                                  1.00 39.34
                                                        56.141
                                                45.119
                                      151.623
                            164
                 CA
                     THR
          1256
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  MOTA
                                                         57.604
                                                                  1.00 40.04
                                                44.805
                                      151.927
                     THR
                             164
          1257
                 CB
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  MOTA
                                                         58.185
                                                                  1.00 45.73
                                      152.625
                                                45.911
                     THR
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                 OG1
          1258
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  MOTA
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                                                                  1.00 45.43
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                                      152.770
                             164
          1259 . CG2
                     THR
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  ATOM
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                                      150.804
                 C
                      THR
                             164
                                                                                     L
          1260
  MOTA
                                                                  1.00 27.93
                                                47.424
                                                         55.597
                                      151.268
                      THR
                             164
                 O
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          1261
                                                                  1.00 29.63
  ATOM
                                                46.349
                                                         56.620
                                      149.584
                      ASP
                             165
                 N
          1262
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  ATOM
                                                                  1.00 37.94
                                                47.533
                                                         56..649
                                      148.739
                      ASP
                             165
          1263
               · CA
                                                                                     L
  MOTA
                                                                   1.00 57.52
                                                         56.673
                                                47.141
                                      147.261
                      ASP
                             165
                 CB
          1264
                                                                                     L
                                                                   1.00 78.24
  ATOM .
                                                         55.352
                                                46.574
                                      146.784.
                             165
          1265
                 CG
                      ASP
   MOTA.
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MOTA	1266	OD1	ASP	165	147.303	47.005		1.00 92.25	L
ATOM .	1267	OD2	ASP	.4165	145.891		55.364	1.00 85.65	L
ATOM ·	1268	C	ASP	165	149.078	48.282	57.923.	1.00 47.66	Ľ
MOTA.	1269	ο΄	ASP	1,65	149.760	47.746		1.00 50.50	L
ATOM	1270	N ·	GLN	166	148.609	49:516	58.030	1.00 47.56	; L
MOTA	1271	CA	GLN	166	148.850	50.319		1.00 42.28	L
ATOM	1272	CB	GLN	166	147.982	51.570	59.185	1.00 44.46	L
ATOM	1273	CG	GLN	166	148.213		60.320	1.00 29.22	r
ATOM	1274	CD	GLN	166	147.967	·53.965	59.885	1.00 17.51	L
ATOM	1275	OE1	GLN .	166	146.909.		59.343	1.00 43.27	r
MOTA	1276	NE2	GLN	166	148.949	54.830	60.103	1.00 25.31	L
MOTA	1277	G.	GLN	166	148.462	49.478	60.422	1.00 38.24	L
ATOM	1278	0	GLN	166	147.361	48.934	60.465	1.00 28.20	L
MOTA	1279	N	ASP	167	149.361	49.364	61.393	1.00 47.65	L
ATOM	1280	CA	ASP.	167	149.072		62.576	1.00:59.05	L
MOTA	1281	CB.	ASP ·	167	150.200		63.591	1.00 40.82	" L
MOTA	1282	CG	ASP .	167	150.022	47.742	64.752	1.00 39.12	L
ATOM.	1283		ASP	167	149.966	46.517	64.510	1.00 57.63	L
ATOM .	1284	QD2	ASP	167 ·	149.927	48.214	65.902	1.00 58.29	L.
ATOM	1285	C	ASP	167	147.768	49.040		1.00 68.64	L L
MOTA	1286	Ö	ASP	.167	147.482	50.237	63.274	1.00 62.87	
MOTA	1287	N	SER	168	146.978	48.079	63.658	1.00.81.22	L
ATOM	1288	CA	SER	168	145.695	48.374	64.271	1.00 77.38	L
MOTA	1289	СВ	SER	168	144.865	47.095	64.370	1.00 77.42	L
ATOM	1290	OG	SER	168	145.397	46.080	63.532	1.00 89.64	L
MOTA	1291	С	SER	168	.145.839	48.994	65.651	1.00 79.26	· L
MOTA	1292	. 0	SER	168 ·	144.922	49.650	66.139	1.00 85.04	L
ATOM	1293	N.	LYS	169	146.990	48.792		1.00 71.82	L L
ATOM	1294	CA	LYS	169	147.210	49.330	67.617	1.00 55.95	
ATOM	1295	CB.	LYS	169	147.785	48.247	68.534	1.00,74.95	L
ATOM -	1296	CG	LYS	,169	147.259		68.253	1.00 84.17	L L
ATOM	1297	CD	LYS	169	148.379		67.762		L
ATOM	1298	CE	LYS	169	147.843		66.885	1.00 85.61	L
MOTA	1299	NZ	LYS	169	148.678		65.665	1.00 81.34	L
MOTA	1300	C	LYS	169	148.114	•	67.658	1.00 46.88	L
ATOM	1301	.0	LYS	169	147.720		68.145	1.00 59.39	r.
MOTA	1302	N	ASP	170 .	149.331			1.00 40.42	Ŀ
MOTA	1,303	CA	ASP	· 170	150.269		67.164	1.00 32.11 1.00 37.35	· L
MOTA	1304	CB	ASP	170	151.647		67.620		L
MOTA	. 1305	CG	ASP	170	152.505		66.479 65.909	1.00 65.81	L
MOTA	1306		1 ASP	170	152.200			1.00 05.01	r _
MOTA			2 ASP	170	153.500	•		1.00 70.13	L
MOTA	1308	,C	ASP	170	150.370		65.856 65.693	1.00 26,65	, L
MOTA	1309	. 0	ASP	170	151.246			1.00 29.78	L
ATOM	. 1310	. И	SER	171	149.466	52.024		1.00 23.70	. L
MOTA	1311	CA		171	149.429		•	1.00 36.91	. T
.ATOM	. 1312	CB	SER	171	148.876			1.00 38.91	L
ATOM	1313	OG		171		54.105		1.00 34.11	,L
MOTA .	1314		SER	171	150.750			1.00 25.60	L
MOTA	1315			171	151.004			1.00 23.80	L
MOTA	1316		THR	172	151.591				
ATOM	1317			172	.152.866			1.00 19.30	L
MOTA	1318	CB	THR	172	154.046	, ,,,,,,,,,	03.123		•

•					•					
ATOM '	1319	OG1	THR	172 .	153.590	50.286	64.039	1.00 61	.43	L
MOTA	1320	CG2	THR	172	154.686	52.449	63.876	1.00 35		L
MOTA	1321	C	THR	172 ·	152.807	50.877 .	61.058	1.00 25	. 7.0	L
MOTA	1322	0	THR	172	151.812	50.189	60.826	1.00 23		·L
MOTA	1323	Ŋ	TYR	173 .	153.892	50.871	60.295	1.00 30	.31	Ľ
MOTA	1324	CA	TYR	173	153.985	50.042	59.109	1.00 21	.84	L
MOTA	1325	CB	TYR	173	154.167	50.911	57.863	1,00 39	.03	L
ATOM	1326	CG	TYR	173	152.916	51.668	57.487	1.00 42	.99	L
MOTA	1327	CD1	TYR	173	151.794	50.994	57.008	1.00 41	.83	L
MOTA	1328	CE1	TYR	173	150.621	51.678	56.709.	1.00 59	•	L
ATOM	1329	CD2	TYR	173	152.834	53.050	57.651	1.00 48		L
MOTA	1330	CE2	TYR	173	.151.663	53.745	57.355	1.00 38	•	L
MOTA	1331	CZ.	TYR	173	150.560	53.052	56.888	1.00 60		L.
ATOM	1332	OH	TYR	·173	149.392	53.723 <sub>.</sub>	56.607			L
MOTA	1333	C .	TYR	173	155.160	49.098	59.245	1.00 30	<del>-</del>	L
ATOM	1334	0	TYR	173	156.089	49.350		1.00 35		L
MOTA	1335	N	SER	174	155.111	48,005	58.505	1.00 26		L
ATOM	1336	CA	SER	174	156.184	47.035	58.539	1.00 25		· L
ATOM	1337	CB	SER	174	155.832	45.874	59.467	1.00 32		: <b>L</b>
MOTA	1338	OĠ	SER	1.74	156.004	46.246	60.824 .	1.00 23		L
	1339	С	SER	174	156.394	46.518	57.136 ·		.29	L,
MOTA	1340	0	SER	174	155 <i>.</i> 475	46.515	56.314	1.00 22		L
MOTA	1341	N .	MET	175	157.614	46.093	56.857	1.00 29		L
ATOM '	1342		MET	175 .	157.925		55.552	1.00 24		L
ATOM	1343	CB	MET	175	158.423	46.693	54.646	1.00 16		L
MOTA	1344	CG	MET'	175	159.379	46.232	53.575	•	.33	r
ATOM	1345	SD	MET	175	159.949	47.595	52.577	1.00 36		L
MOTA	1346	CE	MET	175	160.270	46.761 .		1.00 45		L.
ATOM	1347	C	MET	175 .	158 986	44.498	55.686	1:00 31		. T
MOTA	1348	0	MET	175	159.800	44.522	56.615	1.00 32		L
ATOM	1349	N	SER .	176	158.947	43.544	54.765	1.00 27		L
MOTA	1350	CA	SER ·	176	159.916	42.462	54.737	1.00 33		L
MOTA	1351	CB.	SER	176	159.263	41.137	55.135	1.00 32		L L
ATOM	1352	og	SER	176	159.019	40.331	53.997		.30 .54	L
MOTA	1353 1354	0	ser ser	176 176	160.435 159.669	42.382 42.497	,53.312 52.356	1:00 28		L
ATOM .	1354	И	SER	177	161.743	42.210	53.169	1.00 20		L
ATOM	1356	CA	SER	177	162.355	42.107	51.856	1.00 27		L
ATOM	1357	CB	SER	177	163.231	43.320	51.574	1.00 32		L
ATOM	1358	OG	SER	177 ·	163.713	43.272	50.245	1.00 27		L
ATOM	1359	C	SER	177 .	163.196	40.847	51.802	1.00 22		L
ATOM	1360	o	SER	. 177	164.047	40.621	52.661	1.00 33		L.
ATOM	1361	N	THR	178	162.956	40.026	50.788	1.00 18		L:
ATOM	1362	CA	THR	178	163.687	38.780	50.656	1.00 16		L
MOTA	1363	CB	THR	178	162.740	37.580	50.740	1.00 21		L
ATOM	1364		THR	178	161.938	37.681	51.922	1.00 36		L
ATOM	1365	CG2	THR	178	163.533	36.285	50.782	1.00.22		. L
ATOM	1366	C.	THR	178	164.481	38.675	49.362	1.00 21		L.
MOTA	1367	0	THR.	178	163.949	38.878		1.00 32		L
ATOM		· N	LEU	179	165.764	38.358	49.515	1.00 23		L
ATOM	1369	CA	LEU	179	.166.679	38.183	48.395 .			L
ATOM	1370	CB	LEU	179	168.000	38.899	48.669			L
ATOM	1371	CG.		179	169.043	38.856	47.557 .			L
	· <del>-</del>		- <del>-</del>							

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                                              39.491
                                                       46.291
                                    168.487
                           179
               CD1
                    LEU
 ATOM
         1372
                                                       48.025 - 1.00 24.41
                                    170.289 39.591
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               CD2
                    LEU
         1373
 ATOM
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                                    166.920 36.687
                           179
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                                                        46.941
                                    166.699
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         1377
~· ATOM
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                OG1
                    THR
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                     LEU
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                    LEU
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          1384
                CA
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                                                                 1.00 57.52
                                               33.751
                                                        45.782
                                     171.118
                     LEU
                            181
                CB
  MOTA
          1385
                                                                 1.00 52.16
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                                                        46.126
                                              .35.239
                                     171.097
                            181
                     LEU
                CG
          1386
  MOTA
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                                                                 1.00 64.66
                                                        47.468
                                               35.466
                                     171.777
                CD1 LEU
                            181
          1387
  MOTA
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                                                                 1.00 59.17
                                                        45.032
                                     171.800
                                               36.017
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          1388
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  MOTA
                                                                 1.00 45.72
                                                        45.595
                                               31.558
                                     169.978
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                C
                     LEU
  ATOM .
          1389
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                                                        46.347
                                               30.904
                                     169.250
                            181
                     LEU
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  ATOM
                                                                  1.00 33.32
                                                                                    L
                                                        44.882
                                               31.021
                                     170.964
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                     THR
                N
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  MOTA
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                                               29.601
                                     171.268
                            182
          1392
                 CA
                     THR
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  MOTA
                                                                  1.00 35.79
                                                         43:571.
                                               29.086
                                     171.740
                            182
                 CB
                     THR
          1393
  MOTA
                                                                                    L
                                                                  1.00 51.80
                                                         43.241
                                               29.694
                            182
                                      172.994
                     THR
                 OG1
          1394
                                                                                    L
  MOTA
                                                                  1.00 10.97
                                                         42.497
                                               29.434
                                      170.726
                     THR
                            182
                 .CG2
          1395
  MOTA
                                                                  1.00 31.89
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                                                29.340
                                      172.371
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                 C
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  ATOM
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                             182
                     THR
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                                                28.086
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                                      173.521 27.703 47.326
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                 CA
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                                                        47.492
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                             183
                 CB
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                                      173.959
                                                25.715
                             183
                      LYS
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                                                24.443
                                      174.795
                             183
                      LYS
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                                                24.075
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                      LYS
                 CE
   ATOM
           1403
                                                                  1.00 66.90
                                                         50.151
                                                24.085
                                      176.860
                      LYS
                             183
           1404
                 NZ
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  . ATOM
                                                                  1.00 30.33
                                                         46.750 .
                                                28.168
                                      174.847
                 C
                      LYS
                             183
           1405
                                                                  1.00 47.79
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   MOTA
                                                28.640
                                                         47.462
                                      175.732
                      LYS
                             183
           1406
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   MOTA
                                                        . 45.436
                                                28.044
                                      174.957
           1407
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                             184
                 N
   MOTA
                                                                  1.00 32.28
                                                                                     Τ.
                                                28.422
                                                         44.729.
                                      176.162<sup>.</sup>
                             184
                      ASP
           1408
                 CA
                                                                                     L
   ATOM
                                                                  1.00 41.02
                                                          43.290
                                                27.931
                                      176.089
                             184
                  CB
                      ASP
          · 1409
                                                                                     L
   ATOM
                                                                  1.00 63.85
                                                          43.199
                                                26.424
                                      176.041
                      ASP
                             184
           1410
                  CG
                                                                                     L
   ATOM
                                                          44.147
                                                                   1.00 80.57
                                                 25.754
                                       176.516
                             184
                  OD1 ASP
           1411
   MOTA
                                                                  1.00 76.42
                                                          42.185
                                                 25.907
                                       175.530
                  OD2
                      ASP
                             184
           1412
   MOTA
                                                                   1.00 37.31
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                                       176.443
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                  C
                      ASP
           1413
   MOTA
                                                                   1.00 58.28
                                                          45.547
                                                 30.379
                                       177.250
                      ASP
                              184
                  0
           1414
                                                                                     L
   ATOM
                                                          43.873 . 1.00 33.24
                                                 30.652
                                       175.770
                      GLÜ
                             185
           1415
                  N
   ATOM
                                                                   1.00 36.62
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                                                 32.088
                                                          43.781
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                       GLU
                  CA
   MOTA
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                                                                                     L
                                                          42.702
                                                 32.691
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                             . 185
           1417
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                       GLU
   MOTA
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                                                                                     L
                                                          43.198
                                                 33.484
                                       173.899
                              1.85
                  CG
                      GLU
           1418
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    ATOM
                                                          42.058
                                                                   1.00 78.07
                                                 33.876
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                                       172.973
                       GLU
                  CD
           1419
                                                                                      L
    MOTA
                                                                   1.00 94.70
                                                          41.198
                                                 34.680
                                       173.399
                  OEl
                       GLU
                              185
           1420
    ATOM
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                                                 33.378
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           1421
                  OE<sub>2</sub>
                       GLU
    MOTA
                                                                   1.00 40.77
                                                          45.095
                                                 32.849
                                       175.870
                       GLU
                              185
          .1422
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                                                                    1.00 28.19
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                                                 34:039
                                       176.154
                              185
                       GLU
                  O
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          . 1423
                                                                        45.72
                                                                    1.00
                                                          46.160
                                                 32,171
                                       175.455
                       TYR
                              186
                  N
          . 1424
    MOTA
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•			•						1.00 3	4 42	L
ATOM	1425	CA S	<b>TYR</b>	186		5.357	32.824	47.461	1.00 2		L
ATOM	1426	CB :	ryr	186		4.183	32.284	48.271			L.
ATOM	1427	CG S	<b>TYR</b>	186		4.394	32.396	49.769	1.00		L.
ATOM	1428	CD1 '	TYR	186		4.131	33.590		1.00		L
MOTA		CE1 '	TYR	186.		4.314	33.694	51.833	1.00		L
ATOM	1430	CD2 '	TYR '	186		4.850	31.310	50.509			L
MOTA	1431	CE2	TYR	186	. 17	75.036	31.402.	51.893	1.00		Ĺ
ATOM	1432		TYR	186	17	74.766	32.594	52.549	1.00		L.
ATOM	1433		TYR	186		74.933	32.673	53.913	1.00		L
ATOM	1434		TYR	186		76.641	32.530	48.224	1.00		r .
ATOM	1435	0	TYR .	186	17	77.138	33.358	48.985	1.00		r
MOTA	1436		GLU	187	17	77.163	31.327	48.025	1.00		· L
ATOM	1437		GLU	187		78.380	30.916	48.695	1.00		L
ATOM	1438		GLU	187	17	78.478	29.394	48.707		51.43	T.
ATOM	1439		GLU	187	1.	77.688	28.757	49.831	1.00		L L
ATOM	1440		GLU .	187	1'	77.931	27.269		1.00		P.
ATOM	1441	QE1		187	· 1'	78.505	26.681			72.88	
ATOM	1442		GLU	187	. 1'	77.540	26.690	50.980		92.94	L
ATOM	1443	C	GLU	187	1	79.608	31.516	48.021		25.34	L.
	1444	ō	GLU	187	. 1	80.731	31.319	48.476		33.80	L
MOTA	1445	N	ARG	188	1.	79.393	.32.255	46.937		25.18	L
ATOM	1446	CA	ARG	188	1	80.504	32.887	46.238		28.26	L
MOTA	1447	CB	ARG	188	1	80.430	32.583	44.732		50.64	L
MOTA	1448	CG	ARG	188	. 1	79.374	33.352	43.952		42.62	L
MOTA	_	CD	ARG	188	. 1	79.332	32.895	42.493		43.87	L
ATOM .	145.0	NE	ARG	188	1	79.213	31.440	42.378		93.56	L
MOTA MOTA	. 145.1	CZ	ARG	188	. 1	80.106	30.659	41.779		99.99	. L
	1452	NH1		188	· .1	81.192	31.187	41.230		99.99	Ŀ
MOTA	1453		ARG	188	1	79.918	29.345			99.98	. L
MOTA MOTA	1454	C	ARG	188	. 1	.80.549	34.399			22.65	L L
ATOM	1455	ō	ARG	188	. 1	81.077	35.160			30.16	L
ATOM		N	HIS	189	. 3	L80.00i	34.819			27.86	P.
ATOM	1457	.CA	HIS	189		L79.979				21.88	, L
ATOM	1458	CB	HIS	189	. 3	178.650				40.07	L
MOTA	1459	CG	HIS	189		178.480				47.15	· P
ATOM	1460	CD2	•	189	. :	178.796	38.171			55.79	L
ATOM	1461		HIS	189	1	177.891				63.86	L
ATOM	1462		HIS	189	:	177.849				61.64	L
ATOM	1463		HIS	. 189	:	178.391				29.34	L
ATOM	1464	C	HIS	189		180.152				34.87	
ATOM	1465	. 0	HIS	189		179.750				37.34	
ATOM	1466	N	ASN	190		180.729				47.66	L
ATOM	1467	CA	ASN	190		180.96					L
ATOM	1468	CB	ASN	190		182.388		5 51.795		68.12	· L
ATOM	1469	CG	ASN	190		183.41		7 .50.930		100.00	Ŀ
MOTA	1470	OD:	l ASN	190		183.40				99.97	L
ATOM	1471		2 ASN	190		184.32	0 37.954			99.98	L
ATOM			ASN	190				2 . 52.29		42.97	L
MOTA		_	ASN	190	•	179.38	3 37.79			33.80	L
ATOM			SER	191		179.88				39.67	. T
ATOM			SER	191		179.01				30.33	. L
ATOM	_		SER	19 <b>i</b>		179.69			•	0 31.09	
ATOM		_	SER	191		179.88	7 42.05	6 54.17	7 1.00	0 59.06	
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	•			•				1.00 34.40	L
MOTA	1478	С	SER	191	177.655	40.634	51.967	1.00 34.40	L
ATOM	1479	ο.	SER	191	177.550	40.836	50.753.	1.00 25.05	. T
MOTA	1480	N	TYR	192	176.620	40.574	52.802	1.00 22.04	. L
ATOM	1481	CA	TYR	192	175.246	40.785	52.361	1.00 16.56	r
ATOM	1482	CB	TYR	192	174.420	39.517	52.582	1.00 18.30	ī.
ATOM	1483	CG·	TYR.	192	174.807	38.444	51.598	1.00 33.02	r·
MOTA	1484	CD1	TYR	192	174.383	38.511	_	1.00 33.77	L
MOTA	1485		TYR	192	174.829	37.592	49.330	1.00 36.76	· L
ATOM	1486	CD2	TYR	192	175.683	37.417	51.961	1.00 36.40	L
MOTA	1487	CE2	TYR	192	176.135	36.492	51.024	1.00 38.40	L
MOTA	1488	CZ	TYR	192	175.707	36.587	49.711		L
ATOM	1489	OH	TYR	192	. 176.164.	35.693	48.766	1.00 31.96 1.00 26.50	L
ATOM	1490	C	TYR	192	174.705	41.961	53.160		· L
ATOM	1491	ō	TYR	192	174.749	41.970	54.389	1.00 26.85	Ŀ
ATOM	.1492	И.	THR	1,93	174.205	42.959	52.443	1.00 42.59	L
•	1493	CA	THR	193	173.716	44.165	53.086	1.00 49.57	L
MOTA	1494	· CB	THR	193	174.621	45.362	52.738	1.00 59.55	L
ATOM .	1495	0G1		193	175.983	45.025	53.025	1.00 51.20	r.
ATOM .	1496	CG2		193	174.219	46.592	53.536	1.00 59.94	r r
MOTA	1497	c	THR	193	172.285	44.574	. 52.777	1.00 46.91	
MOTA	1498	<u>o</u> .	THR	193	171.848	44.573	51.621	1.00 57.88	Lí.
ATOM	1499	N	CYS	194	171.578	44.946	53.836	1.00 40.06	L
ATOM	1500	CA	CYS	194	. 170.208	45.409	53.738	1.00 39.66	L
ATOM	1501	C	CYS	194	170.229	46.894	54.090	1.00 50.91	L
MOTA	1501	o	CYS	194	170.419	47.263	55.253	1.00 50.44	L
MOTA		CB.	CYS.	194	169.326	44.652	54.719	1.00 56.36	L·.
MOTA	1503	SG	CYS	194 .	167.606	45.219	54.662	1.00 57.55	L
MOTA	1504	N	GLU	195	170.039	.47.734	53.080	1.00 62.99	·L
MOTA	1505 1506	CA	GLU	195	170.066	49.182	53.262	1.00 56.68	· L
ATOM			GLU	195 .	171.006	49.802	52.231	1.00 67.85	L
MOTA	1507 <sup>.</sup> 1508	CG	GLU	195	171.618	51.121		1.00 75.89	L
MOTA	1509		GLU	195	172.492	51.711			· L
ATOM	1510		1 GLU	195	171.941	52.170		1.00 83.91	r.
MOTA	1511			195	173.731	51.710	51.731	1.00 69.63	r r
MOTA	1512			195	168.689	49.812			· L
MOTA	1512	_	GLU	195	167.926	49.466		1.00 46.93	L
MOTA	1514		ALA	196	168.381				L
ATOM	1515			196	167.085				L
MOTA MOTA	1516			196	166.114				L
ATOM	1517		· ALA	196	167.111				L
ATOM			ALA	196	167.572				Ţi Ti
ATOM	1519		THR	197	166.606	53.748			· L
	1520		THR	197	166.532				L
MOTA ·	1521			197	166.97				L.
ATOM	1522	_	1 THR	197	166.548	55.374		1.00 83.37	ŗ
	1523			197	168.48	5 56.18			L
MOTA		-	THR	197	165.08				L
MOTA MOTA			THR	197	164.15				L
				198	164.90				L
MOTA .				198	163.57	0 56.61			. P
ATOM				198	163.20				L
ATOM				198	161.80	2 55.97			L
ATOM			D2 HIS	198	161.33	3 5628	1 58.61	•	
· MION	2.00							•	

		•		-•		011 ·	56.586	1.00 23.72	L
ATOM · ·	1531	ND1		198	160.691		57.306	1.00 8.26	L.
MOTA	1532	CE1	HIS	198	159.601	• • • • • •	58.545	1.00 26.12	L
MOTA	<b>1533</b>	NE2		198	159.962	56.295	56.001	1.00 65.53	L
ATOM	1534	c ·	HIS	198	163.611	58.101	56.446	1.00 44.38	· L
MOTA	1535	0	HIS	198	164.642		55.776	1.00 69.60	L
MOTA	1536	. N	LYS	.199 ·	162.501	58.804	56.078	1.00 62.83	L
MOTA	1537	CA	LYS	199	162.407	60.235	56.214	1.00 59.10	L
MOTA	1538	CB	LYS	199	160.940	60.665	54.908	1.00 66.79	L
MOTA	1539	CG	LYS	199	160.168	60.725	54.566	1.00 77.11	L
ATOM	1540	CD	LYS	199	159.541	59.376	53.670	1.00 66.29	L
ATOM	1541	CE	LYS	199	160.458	58.543 58.922	52.226	1.00 71.28	r .
MOTA	1542	NZ	LYS	199 .	160.372		57.409	1.00 54.65	L
ATOM	1543	C	LYS	199.	163.100	60:459	57.596	1.00 52.78	L
MOTA	1544	0	LYS	199	163.853	61.418 59.538	58.322	1.00 59.05	L.
MOTA	1545	N	THR ·	200	162.823	59.530 59.542 ^		1.00 72.79	. L
ATOM	1546	CA.	THR	. 200	163.361		60.404	1.00 72.74	L
ATOM	1547	CB	THR	200	162.896	58.262	61.732	1.00 81.55	L
MOTA	1548	OG1	THR	200	162.485	58.594	60.439	1.00 67.03	L
ATOM	1549	CG2	THR	200	164.002	57.222	59.712	1.00 77.51	L
ATOM	1550	C.	THR	200	164.890	59.648	60.785	1.00 76.37	Ľ
MOTA	1551	0	THR	200	165.479	59.774	-58.550		L
ATOM	1552	N	SER	201	165.536	59.607	58.521	1.00 77.00	L
MOTA	1553	CA	SER	.201 '	166.991	59.696	59.082	1.00 70.20	L
ATOM	1554	CB	SER	201	167.599	58.411	59.728	1.00 48.40	L
ATOM	1555	OG	SER	201.	168.828	58.678	57.145	1.00 75.86	L
MOTA	1556	Ċ	SER	201	167.583	59.967 59.436	56.129	1.00 78.72	L
MOTA	1557	0	SER	201	167.126		57.128	1.00 79.38	L
ATOM	1558	M·	THR	202	168.617	60.802	55.897	1.00 85.40	L·
ATOM	1559	CA	THR .	202	169.317		55.942	1.00 82.98	L
MOTA	1560	CB	·THR	202	169.864		57.190	1.00 58.44	L
ATOM	1561	OG:		202	170.53.6	·	55.800	1.00 81.93	L
MOTA	1562			202	168.725		55.752	1.00 87.12	L
ATOM	1563	C	THR	202	170.481		54.697	1.00 90.15	L
ATOM	1564		THR	202.	171.106		56.835	1.00 85.15	L
MOTA	1565	_	SER	203	170.757		56.866		Ľ
MOTA	1566				171.826		58.194	•	L
MOTA	1567		SER	203	172.589		59.041		.L
ATOM	1568			203	172.049		56.719		L L
MOTA	1569	·C	SER	203	171.203 170.682				L
ATOM			SER						L
ATOM			PRO	204.	171.85	=			L
MOTA				204	170.67				L
ATOM				204	171.26			,	.T
MOTA				204	172.26				L
ATOM				204					L
ATOM			PRO	204	172.16			1.00 79.62	L
OTA		_	PRO.	204	169.97				L
OTA			ILE	205	170.17		•		L
1OTA				205	168.86			1.00 59.30	L
ATO				205	169.12			3 1.00 62.73	L
ATO			32 ILE	205 205				3 1.00 51.85	· L
ATO			31 ILE	205	166.91				L
ATO	M 158	3 CI	01 ILE	205	100.91		-		

•								F7 204	1.00 58.53	L
MOTA	1584	C	ILE	205	•	170.711		57.294. 56.241	1.00 60.90	L
ATOM	1585	0	ILE.	205		170.225		57.918	1.00 53.53	L
ATOM	1586	N '	VAL	206		171.719		57.356	1.00 41.22	L
MOTA	1587	CA	VAL	206		172.332		56.810	1.00 18.34	L.
ATOM	1588	CB	VAL	206	•	173.739		56.467	1.00 13.15	L
MOTA	1589	CG1	VAL	206		174.486		55.580	1.00 13.65	. L
ATOM	1590	CG2	VAL	206		173.618	50.706	58.331	1.00 44.96	r.
MOTA	1591	C	LAV	206	•	172.442	48.336 48.517	59.509	1.00 44.72	L
ATOM	1592		VAL	206		172.747	47.137	57.818	1.00 51.44	L
MOTA	1593	· N	LYS	207		172.180	45.915	58.598	1.00 52.57	. Ъ
MOTA	1594		LYS	207		172.269			1.00 54.70	L.
MOTA	1595	CB	LYS	207		170.882	45.438	60.479	1.00 47.68	· L
ATOM	1596	ÇG	LYS	207		170.800	45.036	61.394	1.00 42.68	L
ATOM	1597	CD.	LYS	207		171.141		62.758		L
MOŢA	1598	CE	LYS	207		170.477	44.740		1.00 56.72	L
MOTA	1599	ŃΖ	LYS	207 .		170.763	44.900	57.671	1.00-51.25	L
ATOM	1600	C	LAS .	207		172.906	44.592	56.610	1.00 57.87	L
ATOM	1601	0	LYS	207		172.357	44:396	58.059	1.00 48.56	L
ATOM	1602	·N	SER	208		174.072	43.429	57.230	1.00 44.28	L
MOTA	1603	CA.	SER	208		174.780	44.095	56.525	1.00 43.06	L
ATOM	1604	CB	SER	208		175.956	45.119	•	1.00 64.64	L
ATOM	1605	QG	SER	208		175.511	42.236	58.003	1.00 46.92	. <b>L</b>
ATOM	1606	С	SER	2.08		175.301 175.121	42.129	59.221	1.00 49.18	· L
ATOM	1607	. 0 '	SER	- 208		-	41.342	57.269	1.00 47.47	L
MOTA	1608	N	PHE	209		175.950	40.152	57.850	1.00 48.36	L
MOTA	1609	CA	PHE	209		176.539	39.170	58.296	1.00 58.47	L.
MOTA	1610	CB	PHE	209		175.443 174.804	38.414	57.168	1.00 68.93	L
MOTA	1611	CG	PHE	209.		173.734	38.960	56.471	1.00 77.87	. L
MOTA	1612	CD1		209		175.280	37.161	56.793	1.00 73.00	r
ATOM	1613	CD2		209		173.148	38.270		1.00 71.56	· ' L
MOTA	1614		PHE	209		174.703		55.736	1.00 64.61	L
MOTA	1615	CE2		209		173.633		55.043	1.00 71.74	L
MOTA	1616		PHE	209		177.481		56.851	1.00 44.99	L
MOTA	1617		PHE	209		177.336		55.637	1.00 35.92	L
MOTA	1618		PHE	209		178.463		57.384		L
. ATOM	1619		ASN.	210	٠.	179.444		56.572		L
ATOM	1620		asn	210 210		180.853		.57.064		L
MOTA	1621		ASN	210		181.925		56.112	1.00100.00	L
MOTA	1622		ASN	210		182.386		55.250		L
MOTA	1623			210		182.328		56.258		L
MOTA	1624		ASN ASN	210		179.165		56.741		L
MOTA	1625		ASN'	210	•	178.624		57.763		L
MOTA	1626		ARG	211		179.524		55.756		L
MOTA	1627			211		179.284		5,5 . 872		L
MOTA	1628		ARG	211		179.672		54.576		L
MOTA	1629			211		178.47		53.79		L
ATOM			·	211		178.60	-	52.32		L
ATOM	163					179.36		51.60		L
MOTA	1633		•	211		180.69		51.52		L
MOTA	163	3 CZ	1 ARG			181.41	1 33.377		8 1.00 74.04	L
MOTA				211	•	181.30		50.86		L
ATOM			ARG	211		180.04			0 1.00 78.01	L
MOTA	163	. C				•	•			

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1.00 62.45
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                   ARG
MOTA
        1637
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                                   179.264
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ATOM
        1638
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                                   179.747
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               CA
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        1639
MOTA
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                                   181.065
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               CB
                   ASN
        1640
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                                   181.130
               CG
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        1641.
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                                   180.343
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               OD1
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 MOTA
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                                                                1.00 27.71
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                                    120.401
                                              36.241
                             2
               CG1
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         1648
ATOM
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                                                       64.680
                                                                1.00 34.18
                                    122.281
                                              37.627
                    VAL
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 MOTA
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                                                                1.00 42.92
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                                              35.223
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                             2
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 ATOM
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                                                                1.00 44.59
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                                              35.160
                                    122.610
                    VAL
               CA
         1653
 ATOM
                                                                                  Н
                                                                1.00 45.14
                                                       63.852
                                              34.056
                                    124.382
                    GLN
               N
         1654
 MOTA
                                                                                   Н
                                                                1.00 47.76
                                              .33.990
                                                       63.047
                                    125.594
                    GLN
                CA
         1655
 MOTA
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                                              33.018
                    GLN
                                    126.585
                CB
 MOTA
         1656
                                                                1.00 70.50
                                                                                   Н
                                                       63.226
                                              33.216
                                    128.013
                    GLN
                CG
         1657
 MOTA
                                                                                   Н
                                                       62.768
                                                                1.00 77.13
                                              31.926
                                    128.654
                             3
         1658
                CD
                    GLN
 MOTA
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                                              30.879
                                    128.477
                OEL
                    GLN
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 ATOM
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                                    129.403
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                                    125.324
                    GLN
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                    GLN
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 MOTA
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                     LEU
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          1670
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                                     127.500
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          1671
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                                                                 1.00 47.49
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                                     128.669
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          1672
  MOTA
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                CB
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  MOTA
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                    GLN
  MOTA
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                                                        61.573
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                                                                  1.00 60.41
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                                     127.459
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                                                        57.187
                                               30.379
                              5
                                     128.764
                     GLN
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  ATOM
          1678
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  ATOM
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                 CD
                     GLN
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                                                                  1.00 44.77
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  MOTA
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                                                                  1.00 43.09
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                     GLN
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                 C
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                      SER
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                                    132.464
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                CA
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MOTA
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         1696
                CA
                    GLY
· ATOM
                                                                 1.00 96.74
                                                                                   Н
                                              25.088
                                                        50.046
                                    133.987
                             . 8
         1697
                C
                    GLY
 MOTA
                                                                                   н
                                                                 1.00 99.99
                                                        50.691
                                               25.207
                                    135.032
                              8
                    GLY
 MOTA
         1698
                0
                                                                                   н
                                                                 1.00 99.99
                                                        48.739
                                              .24.757
                                    133.999
                     PRO
                N
 MOTA
         1699
                                                                                   H
                                                                 1.00 99.99
                                     132.851
                                                        47.850
                                               24.529
         1700
                     PRO
                CD
 ATOM
                                                                                   Н
                                                                 1.00 95 17
                                                        .48.047
                                     135.283
                                               24.547
         1701
                     PRO
                CA
MOTA
                                                                1.00 99.99
                                                                                   Ή
                                                        46.702
                                     134.873
                                               23.925
                     PRO
          1702
                CB
 MOTA
                                                                 1.00 99.98
                                                                                   H
                                                        46.852
                                               23.557
                                     133.404
                              9
                     PRO
        , 1703
                CG
 ATOM
                                                                 1.00 83.28
                                                                                   H
                                                        47.872
                                     136.019.
                                               25.882
                              9
                     PRO
                C
        . 1704
 ATOM.
                                                                                   Н
                                                                 1.00 73.84
                                                        47.793
                                     135.387
                                               26.937
                     PRO
                              9
                0
          1705
 MOTA
                                                                                   Н
                                                                . 1.00 73.05
                                                        47.811
                                     137.349
                                               25.847
                             10
          1706
                N
                     GLU
 MOTA
                                                                                    H
                                                                 1.00 56.11
                                                        47.672
                                               27.087
                                     138.109
                             10
                CA
                     GLU
 ATOM
          1707
                                                                                    H
                                                                 1.00 43.53
                                                        48.898
                                     139.003
                                               27.279
                             10
                CB
                     GLU
          1708
 ATOM
                                                                                    Н
                                                                 1.00 30.69
                                               26.554
                                                        50.136
                                     138.487
          1709
                     GLU
                             10
                 CG
 MOTA
                                                                 1.00 42.43
                                                                                    Н
                                                        51.217
                                               27.497
                                     137.988
                             1.0
          1710
                 CD
                     GLU
  MOTA
                                                                                    H
                                                                 1.00 16.81
                                                        51.678
                                               28.352
                                     138.782
                             1.0
                 OEl
                     GLU
          1711
  MOTA
                                                                                    H
                                                                 1.00 22.46
                                               27.374
                                                         51.612
                                     136.803
                             10
                 OE2
                     GLU
          1712
  MOTA
                                                                  1.00 47.28
                                                                                    H
                                               27.223
                                                        46.393
                                     138.939
                             10
                 C
                     GLU
          1713
  MOTA
                                                                  1.00 48.73
                                                                                    Н
                                                         46.017
                                     139.302
                                               28.336
                     · GLU
                             10
          1714
                 O
  MOTA
                                                                  1.00 37.54
                                                                                    H
                                                         45.730
                                                26.106
                                     139.239
                             11
          1715
                 N
                     LEU
  MOTA
                                                                                    н
                                                         44.486
                                                                  1.00 30.14
                                                26.137
                                      140.012
                              11
                     LEU
  ATOM
          17.16
                 CA
                                                                                    H
                                                         44.676
                                                                  1.00 20.14
                                                25.517
                                      141.398
                              11
                     LEU
                 CB
          17.17
  ATOM
                                                                                    H
                                                                  1.00 23.62
                                                         44.045
                                      142.591 26.256
                     LEU
                              11
                 CG
          1718
  ATOM
                                                                  1.00 18.85
                                                                                    H
                                                         43.309
                                      143.477
                                                25,265
                              11
                     LEÚ
                 CD1
          1719
  MOTA
                                                                  1.00 23.67
                                                                                    H
                                                         43.100
                                      142.110
                                                27.357
                              11
                     LEU
                 CD2
          1720
  MOTA
                                                                                    H.
                                                                  1.00 44.95
                                                         43.357
                                                25.400
                                      139.306
                              11
                 C
                      LEU
          1721
  MOTA
                                                                                    Н
                                                         43.519
                                                                  1.00 54.63
                                                24.257
                                      138.867
                 O.
                      LEU
                              11
          1722
  MOTA
                                                                  1.00 41.04
                                                                                    H
                                                         42.207
                                                26.057
                                      139.210
                              12
          1723
                 N
                      VAL
  MOTA
                                                                                    H
                                                                  1.00 44.92
                                                25.466
                                                         41.042
                                      138.564
                              12
                      VAL
           1724
                 CA
  MOTA
                                                                                    н
                                                                  1.00 55.40
                                                26.116
                                                         40.760
                                      137:198
                              12
                      VAL
          1725
                 CB
  ATOM
                                                                                    н
                                                                  1.00 60.33
                                                25.600
                                                         41.736
                                      136.166
                              12
                 CG1
                      VAL
           1726
  MOTA
                                                                   1.00 67.40
                                                                                    н
                                                         40.849
                                                27.631
                                      137.324
                              12
                 CG2
                      VAL
           1727
                                                                                    ·H
  MOTA
                                                                   1.00 38.99
                                                         39.824
                                                25.687
                                      139.428
                              12
                      VAL
  ATOM
           1728
                  C
                                                                                     H
                                                                   1.00 23.16
                                                         39.702
                                                26.727
                              12
                                      140.065
                      VAL
  ATOM
           1729
                 0
                                                                                     H
                                                                   1.00 56.02
                                                         38.928
                                                24.705
                                      139.451
                      LYS
                              13
           1730
                 N
   MOTA
                                                                                     H
                                                                   1.00 61.99
                                                          37.701 .
                                      140.230
                                                24.817
                              13
                  CA
                      LYS
           1731
   ATOM
                                                                                     H
                                                         .37.154
                                                                   1.00 47.53
                                                 23.430
                                      140.577
                              13
                     · LYS
           1732
                  CB
   ATOM
                                                                                     Н
                                                                   1.00 29.92
                                                          37.259
                                                 23.066
                                      142.054
                              13
                      LYS
   ATOM
           1733
                  CG
                                                                                     н
                                                                   1.00 39.21
                                                          36.416
                                                 21.831
                                      142.364
                              13
                      LYS
                  CD
           1734
 ATOM
                                                                   1.00 40.05
                                                                                     H
                                                          35.596
                                       143.629
                                                 22.007
                              13
                      LYS
                  CE
           1735
   MOTA
                                                                                     н
                                                                   1.00 30.64
                                                          36.230
                                       144.804
                                                 21.337
                              13
           1736
                  ΝZ
                      LYŚ
   MOTA
                                                                                     H
                                                                   1.00 60.22
                                                          36.706
                                                 25.595
                                       139.365
                              13
                      LYS
           1737
                  C
  MOTA
                                                                                     H
                                                                   1.00 48.99
                                                 25.287
                                                         36.513
                                       138.184
                               13
                 : 0
                      LYS
           1738
   ATOM
                                                                                     Ħ
                                                                   1.00 55.96
                                                          36.066
                                                 26,619
                                       139.951
                               14
                  N
                       PRO
           1739
                                                                                     Н
   ATOM
                                                                   1.00 55.17
                                                          36.236
                                                 27.003
                                       141.359
                               14
           1740
                  CD
                       PRO
                                                                                     H
   ATOM
                                                          35.091
                                                                   1.00 63.02
                                                 27.477
                                      139.270
                       PRO
                               14
           1741
                  CA
   ATOM
                                                                   1.00 59.73
                                                          34.404
                                       140.412
                                                 28.234
                       PRO
            1742
                  CB
   MOTA
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•		•				22 623	34.929	1.00 60.43	H
ATOM	1743	CĠ	PRO	14	141.685	27.633	34.096	1.00 61.60	H
ATOM	1744	C	PRO	. 14	138.356	26.766	33.275	1.00 63.48	H
ATOM	1745	0	PRO	14	138.802	25.957	34.185	1.00 55.03	H
MOTA	1746	N	GLY	15	137.069	27.093	33.307	1.00 55.23	H
MOTA	1747	CA	GLY	15	136.077	26.503	34.071	1.00 49.69	. н
MOTA	1748	C.	GLY	15	134.961	25.815		1.00 45.93	H
ATOM	1749	0	GLY	15 :	133.800	25.865	33.670	1.00 46.88	Ĥ
ATOM	1750	N ·	THR	16	135.304	25.176	35.182	1.00 46.72	H
ATOM	1751	CA	THR	16	. 134.303	24.480	35.969	1.00 53.32	·H
ATOM	1752	CB	THR	16	134.946	23.549	36.992	1.00 63.69	н
MOTA	1753	OG1	THR	16	135,914	24.275	37.758	1.00 61.76	H
ATOM	1754	CG2	THR	16	135.615	22.387	36.286	1.00 42.84	H
MOTA	1755	C	THR	16	133.361	25.415	36.700	1.00 42.34	н
ATOM	1756	0	THR	16	133.391	26.626	36.505	1.00 46.34	н
ATOM	1757		SER	17	132.535	24.829	37.559	1.00 44.29	H
ATOM	1758	CA	SER	·17	131.543	25.570 *	38.320		н
ATOM	1759	CB	SER	17	130.190	25.458	37.621	1.00 43.09	. н
	1760	OG	SER	· 17	130.349	25.482	36.211	1.00 37.03	н
MOTA MOTA	1761	c	SER	17	131.408	25.051	39.742	1.00 45.39	. н
	1762	ō	SER	17	131.124	23.872	·39.956	1.00 51.18	
MOTA	1763	N	VAL	18	131.599	25.938	40.713	1.00 43.96	<b>н</b>
MOTA	1764	CA	VAL	18	131.483	25.564	42.119	1.00 45.50	н
ATOM	1765	СВ	VAL	18	132.723	25.989	42.932	1.00 47.04	
MOTA	1766	CG		18	132.979	27.469	42.756	1.00 45.76	H
ATOM	1767			18	132.513	25.665	44.400	1.00 36.17	H
MOTA	1768	C	VAL	. 18	130.257	26.218	42.742	1.00 46.62	H
MOTA	176.5	o	VAL	18	.129.772	27.240	42.258	1.00 24.82	H
ATOM	1770	И.		19	129.758	25.610	43.813	1.00 53.11	H
MOTA	1771	CA	ARG	.19	128.589	26.122	44.518	1.00 58.98	H
MOTA	1772	CB	ARG	19	127.414	25.157	44.354	1.00 48.17	н
MOTA	17.73	CG		19	126.252	25.443	45.280	1.00 32.81	H
MOTA	1774			19	125.479	24.167	45.605	1.00 61.51	H
MOTA	1775			19	126.212	23.302	46.530	1.00 70.76	H.
ATOM	1776			19	125.661	22.352	47.283	1.00 68.17	·H
MOTA	177.7		1 ARG	19	124.353	22.124	47.232	1.00 41.10	H
MOTA	1778			19	126.428	21.625	48.090	1.00 47.54	н
MOTA	1779		ARG	19	128.912	26.282	46.000		H
MOTA	. 1780		ARG	19	129.050				• Н
ATOM	1781		ILE	20	129.043	27.523			· H
MOTA	1782		_ •	20 .	129.345	27.780			
ATOM	1783			20	130.052	29.137	48.067		H
MOTA	1784			20	131.474	29.053			H
ATOM	1789			20	129.280	30.243			
ATOM	1786	י כנ	)1 İFE	20	129.929	31.606	47.466		H.
MOTA			ILE	20	128.059	27.800			'H
ATOM			ILE	20	126.960	27.764			~ H
MOTA			SER	21	128.208	27.860	49.98		H
MOTA				21	127.058	27.892	50.863		
MOTA				21	126.810				H H
MOTA			_	21	127.562	26.314			
MOTA				. 21	127.260	28.917			. Н
MOTA					128.28			5 1.00 70.39	· H
MOTA '				22	126.26	2 29.01	3. 52.83	9 1.00 69.21	
MOTA		٠				•			

	_				•				1.00 6	1 94		H
MOTA	1796	CA .	CYS	22		6:263	29.940	53.963	1.00 5		٠	H
ATOM		С	CYS	22		4.996	29.635	54.745	1.00 5			H
ATOM	1798	0	CAR .	22		3.890	29.845	54.249	1.00 5			Н.
ATOM	1799	CB	CYS	22	12	6.233	31.379	53.461	1.00			н
ATOM	1800	SG	CYS	22	1.2	5.483	32.535	54.637	1.00 4			н .
ATOM	1801	N	GLU	23		5.154		55.968				H
	1802	CA	GLU	23 .	12	3.998	28.783		1.00			H
ATOM	1803	CB	GLU	23	12	24.140	27.339		1.00			н.
MOTA	1804	ÇG	GLU	23	1.2	25.578	26.915		1.00			H
MOTA		CD	GLU	23		25.807	26.370	58.853	1.00		•	
MOTA	1805		GLU	23		24.810	26.025	59.525	. 1.00			H
MOTA	1806			23	12	26.982	26.286	59.278	1.00			H
ATOM	1807		GLU	23 .		23.723	29.675	57.962		47.05	•	H
MOTA	1808	Ç	GLU	23		24.610	29.940	58.777		50.01		, н
MOTA	1809	Ó	ALA	24		22.472		58.060		39.44		H
ATOM	1810	N.		24		22.022		59.143		43.91		H
MOTA	1811	CA	ALA	24		20.770				40.39		H
MOTA	1812	CB	ALA			21.745				49.01		H
MOTA	1813	C	ALA	24	. 1	21.72	28.983			44.02		· H
MOTA	1814	0	·ALA	24		21.752				60.65		H
MOTA	1815	N	SER	25		21.504			1.00	64.10		H
MOTA	1816	CA	SER	25		.22.557				76.12		H
MOTA	1817		SER	25		.22.337				87.44		H
ATOM	1818	OG	SER	25		.23.782				53.28		H
MOTA	1819	C	SER	25						50.41	•	H
MOTA	1820	0	SER	25		22.520	•			46.94		H
ATOM	1821	N	$\mathbf{GLY}$	26		20.384	_			30.92		H
ATOM	1822	CA	GLY	. 26		20.275				32.69		н
ATOM	1823	C	GLY	26		119.04	•	• -		19.54		H
ATOM	1824	0	GLY	26		118.71				42.28.	•	H
MOTA	1825	N.	TYR	27		118.37				45.58		H
ATOM	1826	CA	TYR	27		117.16	·			51.85		Ĥ
ATOM	1827	CB	TYR	· 27		117.54		-	_	59.01		H
MOTA	1828	CG		. 27		118.02				52.27		H
MOTA	1829	CD	1 TYR	27		117.15				42.40		н
ATOM	1830	CE	1 TYR	.27		117.59		. —	_	52.66	•	H
ATOM	1831	CD	2 TYR	27		119.35				46.26	•	н
ATOM	1832	CE	2 TYR	27		119.80				50.61	•	H
ATOM	1833	CZ	TYR	27		118.91				42.85		H
ATOM	1834	OH	TYR	27		119.36				48.20		H.
ATOM	1835		TYR	.2.7		116.25				30.85		н
ATOM	1836		TYR	27		116.55				47.35		H
ATOM	1837		THR	28		115.13				0 41.83		н
ATOM	1838		THR	28		114.17		88 61.77	1 1 0	39.96		н
ATOM	1839			28		112.78				0 50.93		• н
ATOM	1840		1 THR	28		112.27				0 45.16		H
ATOM			32 THR	28		111.83				0 40.89		н
ATOM				28	•	114.6				0 31.24		н
ATOM			THR	28		114.6				0 41.61		н
ATOM				29		115,0				0 41.45		H
ATOM				29	•	115.5				0 30.51		H
ATOM						115.9				0 30.31		н
ATOM							11 30.4			0 30.37		, н
			D1 PHE	29		117.8	33 31.0	65 56.43	39, 1.0	. 30.37		
ATOM					,							•

	••				•			1.00 36.28	H
MOTA	1849	CD2	PHE	29	116.032		55.700	1.00 38.28	. н
ATOM .	1850	CE1	PHE	29	118.469		55.214	1.00 41.18	H
MOTA	1851	CE2	PHE.	29	116.666	29.500	54.463	1.00 35.05	H
MOTA	1852	CZ	PHE	29	117.889	30.122	54.225	1.00 54.24	H
MOTA	1853	C	PHE	29			57.379	1.00 54.24	н
MOTA	1854'	0	PHE	· 29	114.952	33.331	56.480	1.00 55.99	н
ATOM	1855	N	THR	30 .	113.342	32.164	57.527	•	, H
ATOM	1856	CA	THR	30 ·	112.276	32.557	56.615	1.00 52.36 1.00 53.76	н
ATOM	1857	CB	THR	30 .	111.052 <sup>.</sup>	31.652	56.824		н.
ATOM	1858	OG1	THR	30	110.733	31.583	58.225	1.00 35.56	H
ATOM	1859	CG2	THR	30	111.357	30.244	56.304	1.00'44.72	н.
ATOM	1860	С	THR	30	111.829	34.016	56.703	1.00 47.50	H
ATOM	. 1861	0	THR	30	110.914	34.426	55.996	1.00 53.11	H
ATOM	1862	.N	SER	31	112.470	34.804	57.554	1.00 46.37	Н
MOTA	1863	CA	SER	31	112.094	36.207	57.697	1.00 45.74	H.
ATOM	1864	CB	SER.	31	111.832	36.521		1.00 29.27	H.
MOTA	1865	OG	SER	3,1	110.583	37.159	59.337	1.00 47.69	
	1866		SER	31	113.143	37.175	57.150	1.00 47.78	H
MOTA	1867	o	SER	31	113.149	38.358	57.509	1.00 46.57	H
MOTA	1868	N	TYR	32	114.027	36.683	56.286	1.00 31.83	H
ATOM	1869	CA.	TYR	32	115.068	37.530	55.720	1.00 30.55	н.
MOTA	1870	CB	TYR	32	116.287	37.556	56.642	1.00 32.62	. Н
MOTA	1871	CG	TYR	32	116.075	38.248	57.963	1.00 37.51	H
MOTA MOTA	1872	CD1		32	115.494	37.579	59.031	1.00 33.89	. H
	.1873	CEI		32	115.358	38.184	60.266	1.00 35.72	H
MOTA	1874		TYR	32	116.510	39.556	58.166	1.00 39.03	H
MOTA	1875	CE2		32	116.378	40.173	59.401	1.00 40.85	H
MOTA	1876	cz	TYR	32	115.803	39.476	60.449	1.00 43.40	H
ATOM	1877	OH	TYR	32	115.693	40.053	61.695	1.00 55.17	H
MOTA	1878	C	TYR	32	115.526	37.071	54.342	1.00 42.11	H
MOTA	1879	Ö	TYR	32	115.438	35.889	54.012	1.00 37.33	н
MOTA	1880	N	TYR	33	116.021	38.017	53.545	. 1.00 52.12	H
ATOM.	1881	ĊA	TYR	33	116.544	37.721	52.210	1.00 50.02	H
MOTA	1882	СВ	TYR	33	. 116.576	38.960	51.309	1.00 42.85	H
MOTA	1883	CG	TYR	33 .	115.263	39.601	50.944	1.00 58.80	H
MOTA	1884		1 TYR	33	114.637	39.313	49,730	1.00 66.77	H
MOTA .	1885		1 TYR		113.466	39.968	49.345	1.00 69.61	H.
MOTA	1886		2 TYR	33	114.683	40.558	51.771		H
MOTA	1887	CE		33	113.513	41.220			H
MOTA MOTA	1888	CZ		33	112.909	40.921	50.185		Н
	1889			33	111.746	41.574	49.830	1.00 56.44	H
MOTA	1890		TYR	33	118.000	37.359	52.441		. Н
MOTA	1891		TYR	33	118.601	37.825	53.411		H
MOTA	1892		, ILE	34	118.574	36.538	51.570	1.00 39.36	H
MOTA	1893			34	119.991	36.237	51.705		H
MOTA	1894			34	120.310	34.720	51.687	1.00 41.72	H
MOTA	1895			34	121.831	34.515			H
ATOM	1896		1 ILE	34	119.647				H
MOTA	1897		1 ILE	34	120.435	34.137	54.17		Н
MOTA		•	ILE	34	120.629	36.900			H
MOTA			ILE	34 ·	120.304	36.568	49.35	1.00 36.71	. н
MOTA			HIS	35	121.506	37.864			H
MOTA				35	122.185	38.573	49.66	1.00 29.41	. H
MOTA	190.			_		• •			

	•					40 063	49.990	1.00 22.47	H
ATOM	1902	CB	HIS	35	122.300		50.047	1.00 28.34	H
ATOM ·	1903	CG	HIS	35	120.983		51.049	1.00 17.42	H
MOTA	1904		HIS	35	120.082	41.427	48.965	1.00 34.24	H
MOTA	1905		HIS	35 .	120.446	41.427	49.298	1.00 35.85	. H
MOTA	1906	CE1	HIS	35 ·	119.266		50.556	1.00 28.90	н
MOTA	1907	NE2	HIS	35	119.023		49.482	1.00 24.58	H.
ATOM	1908	C	HIS	35 .	123.574	38.000	50.403	1.00 40.74	. н
ATOM	1909	0	HIS	35	124.156	37.437	48,282	1.00 18.85	н
MOTA	1910	N	TRP	. 36 :	124.104		47.984	1.00 25.49	H.
ATOM	1911	CA	TRP	36	125.430	37.664	47.104	1.00 38.00	н
ATOM	1912	ÇB	TRP	36	125.334	36.410		1.00 42.56	H
ATOM	1913	CG	TRP	36	125.226	35.122	47.882	1.00 28.82	н
ATOM	1914	CD2	TRP	36	126.288	34.433	48.564	1.00 28.62	н
ATOM	1915	CE2		36	125.730	33.274	49.146	1.00 18.87	н
MOTA	1916	CE3		36	127.658	34.687	48.737	1.00 40.81	н
ATOM '	1917		TRP	36	124.097	34.368	48.075	1.00 30.56	н
MOTA	1918	NE1	•	36	124.394	33.257	48.834		H
	1919	CZZ		36	126.492	32.368	49.889	1.00 44.00	H,
MOTA	1920	CZ3		36 ·	128.418	33.786	49.479	1.00 41.71	. н
MOTA	1921	CH2		36	127.832	32.641	50.045	1.00 49.64	H
MOTA	1922	C	TRP	36	126.189	38.784	47.269	1.00 22.21	- н
MOTA	1923	ō	TRP	36	125.658	39.410	46.352	1.00 20.33	. н
MOTA		N	VAL	37	127.420	39.044	47.703	1.00 21.22	H
MOTA		CA	VAL	37	128.237	40.085	47.089	1.00 29.63	
MOTA	1925	CB	VAL	.37	128.157	41.414	47.887	1.00 30.69	H
MOTA	1926		1 VAL	37	126.874	41.453	48.701	1.00 7.82	H
MOTA	1927	CG		37	129.366	41.569	48.780	1.00 16.02	H
MOTA	1928		VAL	37	129.693	39.641	46.984	1.00 33.49	H .
MOTA	1929	C		. 37	130.223	39.017	47.900	1.00 17.14	H
MOTA	1930	0	LYS	38 .	130.330	39.970	45.862	1.00 43.70	H
MOTA	1931	•		38	131.720	39.591	45.619	1.00 47.72	н
MOTA	1932	CA		38	131.849	38.932	44.233	1.00 55.60	H
ATOM	1933			38	132.592		43.175	1.00 55.19	H
ATOM	1934			38	133.109		42.022	1.00 50.50	• н
MOTA	1935			38	131.967	•	41.155	1.00 51.42	H
ATOM	1936		_	38	132.372		40.335	1.00 38.13	н.
MOTA	1937			38	132.699		45.732		H
MOTA	1938		LYS	38	132.467			1.00 52.35	H
MOTA	1939		LYS GLN	39	133.798		46.439	1.00 38.36	H
MOTA	1940			39	134.819		46.621		. н
MOTA	1941			39	134.969				H
MOTA	1942			39	136.078		48.409		н
ATOM	1943			39	135.965			1.00 27.61	• н
MOTA	1944	CI		. 39	135.386			1.00 26.42	H
MOTA	1945		E1 GLN	39	136.517			1.00 31.89	H
MOTA	1946		E2 GLN	39.	136.142			1.00 29.22	H
MOTA				39	136.78			2 1.00 19.00	H
MOTA		•		40	136.54			3 1.00 41.18	н
MOTA					137.79		44.31		н
ATOM					127 90			9 1.00 47.54	H
MOTA				40 40	137.20			3 1.00 39.67	H
ATOM			G ARG		137.40			8 1.00 63.74	. н
ATOM			D ARG	40	138.76				н
ATOM	195	4 N	E ARG	40	1000	- , - · · ·		•	

					139.215	39.178.	39.816	1.00 59.13	H
MOTA	1955	CZ	ARG	40	139.215	38.137	40.046	1.00 49.49	. н
MOTA	1956	NH1		40		38.982	39.400	1.00 64.52	H.
MOTA	1957		ARG	40	140.459	41.791	45.024	1.00 49.05	. н
MOTA	1958	C	ARG	40	138.971	42.989	45.312	1.00 41.67	. н
MOTA	1959	0	ARG .	. 40	138.955		45.329	1.00 49.95	. н
MOTA	1960	N	PRO	41	140.007	40.996	45.022	1.00 60.26	H.
ATOM	1961	CD.	PRO	41	140.102	39.557		1.00 40.75	н
MOTA	1962	CA	PRO	41	141.200	41.485	46.013	1.00 50.53	. н
ATOM	1963	CB	PRO	41	142.268	40.476	45.625	1.00 62.82	н
ATOM	1964	. CG	PRO	41	141.516	39.202	45.415	1.00 38.02	· н
MOTA	1965	С	PRO	41	141.558	42.888	45.576	1.00 47.09	. н
ATOM	1966.	0	PRO	41	141.769	43.147	44.392		H
ATOM	.1967	N	GLY	42	141.614	43.794	46.542	1.00 36.72	H
ATOM	1968	CA	GLY	42	141.952	45.170	46.241	1.00 31.35	H
ATOM	1969	· C	GLY.	42	140.726	45.981	45.900	1.00 40.05	н
ATOM	1970	ο.	GLY	42	140.468	47.014		1.00 41.40	H
MOTA	1971	N .	GLN	43	139.975	45.502	44.913	1.00 58.75	
ATOM	1972	CA	GLN	43	138.752	46.163	44.468	1.00 67.06	Н
ATOM	1973	CB.		43	138.192	45.449	43.227	1.00 64.21	H
ATOM	1974	CG	GLN.	43	137.035	46.178	42.540	1.00 71.56	H
MOTA	1975	CD	GLN	43	135.900	`45.251	42.130	1.00 71.51	H
ATOM	1976	OE1		43	i35.330	44.540	42.963	1.00 67.00	H
ATOM	1977	NE2		43	135.566	45.255	40.842	1.00 53.00	н
	1978	C	GLN	43	137.701	46.158	45.581	1.00 68.90	H
MOTA	1979	. 0	GLN .	43	137.782	45.366	46.521	1.00 72.87	H.
MOTA	1980	N	GLY	44	136.723	47.055	45.471	1.00 67.47	H
ATOM		CA	GLY	44	135.661	47.119	46.458	1.00 54.03	H
ATOM	1981	C	GLY	44	134.746	45.927	46.268	1.00 52.55	H.
MOTA	1982	0	GFX	44	135.191	44.881	45.794	1.00 65.13	H
MOTA	1983	N	LEU	45	133.474	46.062	46.623	1.00 38.94	н
MOTA	1984	CA	LEU	45	132.552	44.946	46.456	1.00 50.12	H
MOTA	1985		LEU	45	132.197	44.339	47.819	1.00 44.25	H
MOTA	1986	CB	LEU	.45	131.306	45.109	48.790	1.00 36.87	H
ATOM	1987		LEU	45	131.661	44.692	50.212	1.00 34.38	H
ATOM	1988		LEU	45	131.480	46.605	48.597	1.00 31.30	H
MOTA	1989		LEU	45	131.283	45.315	45.689	1.00 47.35	H
MOTA	1990	C ·		45	130.876	46.475	45.656	1.00 52.97	H
ATOM	1991	0	GLU GLU	45. 46	130.673	44.311	45.066	1.00 38.18	H
MOTA	1992	N		46	129.468	44.497	44.275	1.00 32.36	, H
MOTA	1993	· CA	GLU	46	129.779	44.312	42.787	1.00 54.58	H
MOTA	1994	•	GLU		131.106		42.502	1.00 70.14	. H
MOTA	1995			•	131.544	43.722			· H
ATOM	1996		GLU	46 46	132.769	43.760	40.796	1.00 60.49	H
MOTA'	1997				130.660				H
MOTA	1998	•	2 GLU	46	128.400				H
MOTA	1999		GLU	46	128.697				H
ATOM.	2000		GLU.	46	127.157				H
MOTA	2001		TRP	47	127.137				H
MOTA	2002			47	124.794				H
. ATOM	2003			47	123.538				н
MOTA	2004			47	122.417				H
ATOM	2005			47 .	121.440	•			H
MOTA	2006			. 47.	122:148				H
MOTA	2007	CE	3 TRP	47.	152.140			•	ě

					٠,		'	1.00 44.85	. Н
ATOM	2008	CD1	TRP	47	123.204		46.547	1.00 44.22	H
MOTA	2009	NE1	TRP	47	121.942		46.533	1.00 48.68	н.
MOTA	2010	CZ2	TRP	47	120.205			1.00 48.92	н
MOTA	2011	CZ3	TRP	47 .	120.924	-	42.597	1.00 48.32	H
ATOM	2012	CH2	TRP ·	47	119.969	42.073	43.420	1.00 35.77	н
ATOM	2013	C	TRP	47	125.692	41.936		1.00 45.19	Н
MOTA	2014	· 0	TRP	47	125.359	42.260	42.449	1.00 45.19	н н
MOTA	2015	N	ILE	48	125.800	40.671		1.00 45.61	н Н
ATOM	2016	CA	.ILE	48	125.529	39.562	43.080		. н
ATOM	2017	CB	ILE	48	126.185	38.266		1.00 25.87	. H
ATOM	2018	CG2	ILE	48	125.479	37.039		1.00 23.09	н
ATOM	2019	CG1		48	127.657	38.249	43.202	1.00 15.27	. н
ATOM .	2020	CD1		48	128.449	37.133		1.00 20.12	н
MOTA	2021,	C	ILE	: 48	124.028	39.356	42.936	1.00 35.05	<u>н</u> . Н
ATOM	2022		ILE .	48	123.461	39.591	41.870	1.00 41.96	H
ATOM	2023	N	GLY	49	123.388	.38.918 ~	44.013	1.00 32.61	н
ATOM	2024	CA	GLY	49	121.953	38.689	43.986	1.00 30.75	
	2025	C	GLY	49	121.432	38.298		1.00 38.37	н
ATOM	2026	ō	GLY .	49	122.161	38.327	46.349	1.00 41.94	H
MOTA	2027	N	CYS .	50	120.163	37.931	45.431	1.00 37.54	H
ATOM	2028	CA	CYS	50	119.587	37.540	46.705		Н
ATOM: ATOM	2029	CB	CYS	50	119.095	38.774	47.462	1.00 51.77	H
	2030	SG	CYS	50	117.500	39.407	46:877	1.00 50.59	H
ATOM	2031	_	CYS	50 ·	118.438	36.577	46.500	1.00 42.42	H
MOTA	2032	0	CYS	. 50	117.835	36.535	45.431	1.00 50.09	H
MOTA	2032	N.	ILE	51	. 118.146	35.804	47.537	1.00 42.92	H
ATOM	2034	CA	ILE	51	117.059	34.837	47.502	1.00 37.44	H
ATOM	2035	CB	ILE	51	117.596	.33.380	47.377	1.00 28.69	H
MOTA	2036	CG2		51	118.648	33.111	48.440	1.00 29.15	H
ATOM ATOM	2037	CGI		51	116.448	32.382	47.521	1.00 22.13	H
	2038	CD		· 51	115.840	31.963	46.201	1.00 43.28	H
MOTA .	2039	C C	ILE	51	116.277	34.989	48.800		н
ATOM	2040	ō.		51	116.861	35.219		1.00 34.19	Н
•	2040	N.	TYR	- 52	114.957	34.886	48.706	1.00 38.73	• н
MOTA	2042			52	114.124	35.013	49.888	1.00 34.95	. н
MOTA	2043	CB	TYR	52	112.954	35.960	49.643	1.00 26.98	Н
MOTA	2044	CG	TYR	52	112.041	36.049	50.840	1.00 28.39	н
ATOM		CD		52	112.571	36.155	52.132	1.00 31.39	н
ATOM .	2045			52	111.752	36.193	53.244	1.00 43.44	н
MOTA	2047	•		52	110.660	35.986	50.695	1.00 19.91	. Н
MOTA MOTA	2048	•	2. TYR	52	109.821	36.022	51.800·	1.00 43.98	. н
	2049			52	110.376	36.124	53.075	1.00 56.97	. н
MOTA	2050			52	. 109.556	36.153	54.178	1.00.67.54	н
MOTA	2051			52	113.578		50.350		H
MOTA	2052		TYR	_	112.611	33.161			. н
MOTA	2053		PRO	53	114.191	33.092			H
MOTA	2054		•	53	115.347	33.610			H
MOTA	2055			53	113.728	31.803			H
ATOM			•	53	114.599	31.566			· H
MOTA	2057			53	115.817	32.404			. H
MOTA			PRO	53	112.279	31.971			
MOTA MOTA	2059	•	_	53	111.926	32.927			H
MOTA			GLY	54	. 111.44	31.055	51.815	1.00 43.54	H
ATON				•					•

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1.00 53.47
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                                                       52.120
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ATOM
        2061
               CA
                    GLY
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                                                       50.860
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                    GLY
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MOTA
        2062
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                                              29.936
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                    GLY
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ATOM
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ATOM
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ATOM
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ATOM
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                                                                 1.00 59.93
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                                              31.536
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                    VAL
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               CG1
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· ATOM
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                                    113.110
                     ASN
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                                               35.465
                                     114.974
                             58
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                CA
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                OG1
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                                               33.516
                                                         42.314
                                     114.628
                             58
                CG<sub>2</sub>
                     THR
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                CG
         2097
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          2104
  ATOM
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  MOTA
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          2107
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                              60
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                 CD2
                      TYR
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                                                                  1.00 47.25
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                                                         40.217
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                                      118.077
                 CE<sub>2</sub>
                      TYR
  MOTA
          2109
                                                                                     Н
                                                                  1.00 51.22
                                                33.647
                                                         40.469
                                      119.033
                              60
          2110
                 CZ
                      TYR
  MOTA
                                                                                     H
                                                                   1.00 56.18
                                                         40.883
                                                32.391
                                      118.621
                              60
          2111.
                 OH
                      TYR
  MOTA
                                                                   1.00 25.63
                                                                                     H
                                                          39.618
                                                40.034
                                      120.367
                              60
          2112
                ٠C
                      TYR
  MOTA
                                                                   1.00 17.78
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                                                          39.008
                                                40.746
                                      119.574
                              60
                      TYR
  ATOM
          2113
                 0
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							20 770	1.00 31.77	H	
ATOM	2114	N	ASN	61 .	121.645	40.354	39.789		H	
ATOM'	2115	CA	ASN	61	122.224	41.551	39.213	1.00 30.42	н	
ATOM	2116	CB	asn	<b>61</b> .	123.542	41.891	39.907	1.00 26.96	H	
MOTA	2117	CG	ASN	. 61	124.176	43.155	39.367	1.00 28.98		
MOTA	2118	OD1	ASN	. 61	124.721	43.964	40.120	1.00 39.03	Н	
ATOM	2119		ASN	. 61	124.105	43.335	38.052	1.00 39.88	н	
ATOM	2120	С	ASN	61	122.480	41.102	37.787	1.00 42.86	Н	
ATOM	2121	0	ASN	61	123.062	40.041	37.571	1.00 56.00	, H	
MOTA		N	GLU	62	122.045	41.889	36.812	1.00 46.51	H	
ATOM	2123	•	GLU	62	122.224	41.498	35.424	1.00 52.07	H	•
ATOM	2124	CB	GLÜ	62	121.511	42.490	34.504	1.00 57.39	H	
ATOM	2125	CG	GLU	62	120.513	41.839	33.531	1.00 76.62	H	
ATOM	2126	CD	GLU	<sup>`</sup> 62	119.280	41.242	34.214	1.00 81.14	H	
	2127		GLU	62	119.442	40.484	35.197	1.00 79.43	H	
MOTA	2128		GLU	62	118.148	41.528	33.759	1.00 70.90	H	
MOTA	. 2129	C	GLU	62	123.678	41.327	35.000	1.00 53.65	H	
MOTA		0	GLU	62	123.953	40.991	33.847	1.00 75.05	н	
MOTA	2130	N	LYS	63	124.610	41.543	35.922	1.00 36.05	H	
MOTA	2131	CA.	LYS	63	126.025	41.379	35.604	1.00 35.02	H	
MOTA	2132		LYS	63	126.862	42.421	36.353	1.00 26.34	H	
MOTA	2133	CB	LYS	63 ·	127.215	•	35.532	1.00 49.15	· H	
ATOM	2134	CG	LYS	63	126.773		36.217	1.00 45.62	H	
MOTA	2135	CD		63 <i></i>	127.938	45.619	36.920	1.00 40.94	H	Ĺ
MOTA	2136	CE	LYS	63	128.652		37.772	1.00 39.59	H	]
ATOM	2137	NZ	LYS	63	126.506		35.961	1.00 40.58	H	]
MOTA	2138	C .	LYS	63	127.618	39.576	35.611	1.00 45.93	H	Ι.
MOTA	2139	0	LYS	64	125.657	39,214	36.658	1.00 47.98	E	1
ATOM	2140	N	PHE	64	125.975	37.849	37.073	1.00 42.86	F	1
MOTA	2141	CA	PHE		126.263	37.789	38.579	1.00 42.85		ַ 1
MOTA	2142	CB	PHE	64	127.177	38.872	39.068	1.00 44.03	F	I
MOTA	2143	CG	PHE	64	128.538	38.831	38.791	1.00 50.59	F	Ţ
MOTA	2144		PHE	64	126.680	39.929	39.817	1.00 38.08	·	I.
MOTA	2145		PHE		129.388	39.830	39.255	1.00 45.27	F	I
MOTA	2146		PHE	. 64		40.933	40.284		I	I
ATOM	2147	CE2		64	127.524	40.883	40.004	1.00 31.11	I	Ŧ
MOTA	2148	CZ	PHE	64	128.877	36.908	36.768	1.00 43.11	· I	1
MOTA	.2149	C	PHE	64	. 124.823	35.988	37.535	1.00 47.33	I	1
MOTA	2150	0	PHE	. 64	124.560	37.128	35.644	1.00 55.21	•	H
ATOM.	2151	N	LXS	65 .	124.148	36.302	35.259	1.00 59.07	. 1	H
ATOM.	2152	CA	LYS	65	123.005			1.00 45.97	. 1	H
MOTA	2153	CB	LYS	65	122.383		33.251			H
ATOM	2154	CG	LYS	65	123.146	37.914	32.270			H
ATOM	2155	CD	LYS	65	124.165	37.363	31.811	1.00 50.30		H
MOTA	2156	CE	LYS	65	125.116	38.461	30.398	1.00 58.93	1	H
MOTA	2157	NZ	LYS	65	125.548	38.271 34.802				н
MOTA	2158	C.		65	123.279				•	H
ATOM	2159	0	LYS	65	122.598					Н
MOTA	2160		ASP	66	124.267					H
MOTA .	2161		ASP	66	124.579					H
MOTA	2162			66	125.508					H
MOTA	2163		ASP	66	124.747					H
MOTA	2164		1 ASP	66	124.869					H
MOTA	2165		2 ASP	66	124.023					H
MOTA	2166	C	ASP	66	125.168	32.265	.35.251	. 1.00 /0.23		

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35.792
                                             31.365
                           66
               0
                   ASP
MOTA
        2167
                                                                                  H
                                                                1.00
                                                                      62.38
                                             32.605
                                                       35.637
                                   126.399
                   LYS
                           67
               N
        2168
MOTA
                                                                                  H
                                                                1.00 49.02
                                                       36.750
                                             31.934
                                   127.071
               CA
                   LYS
                           67
        2169
ATOM
                                                                                  H
                                                                1.00 25.39
                                                       37.115
                                              32.653
                                   128.374
                            67
        2170
               CB
                   LYS
MOTA
                                                                1.00 48.63
                                                                                  H
                                                       36.489
                                   128.541
                                              34.034
                   LYS
                            67
               CG
        2171
MOTA
                                                                                  Н
                                                       36.675
                                                                1.00 21.16
                                              34.579
                                   129.958
                   LYS
                            67
               CD
ATOM
       · 2172
                                                                                  H
                                                                1.00 43.17
                                              34.018
                                                       35.624
                                    130.912
                            67
               CE
                   LYS
       .2173
MOTA
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                                                       36.179
                                                                1.00 34.20
                                             33.618
                                   132.251
               NZ
                   LYS
                            67
        2174
MOTA
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                                              31.887
                                                               1.00 59.48
                                                      .37.977
                                    126.178
                            67
        2175
               C
                    LYS
MOTA
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                                             30.816
                                                                1.00 51:12
                                                       38.390
                                    125.721
                            67
                    LYS
ATOM
        2176
               0
                                                                                   Н
                                                                1.00 67.14
                                                       38.545
                                              33.066
                                    125.929
                            68
                    ALA
        2177
               N
ATOM
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                                                                1.00 54.74
                                              33.220
                                                       39.741
                                    125.104
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        2178
                    ALA
               ÇA
MOTA
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                                                                1.00 54.84
                                                       40.108
                                              34.688
                                    125.017
                            68
        2179
               CB
                    ALA
MOTA
                                                                1.00 49.40
                                                                                   Н
                                                       39.631
                                              32.631
                                    123.701
                            68
                    ALA
MOTA
        2180
               C
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                                                                 1.00 58.08
                                                       38.896
                                              33.136
                                    122.851
                    ALA
                            68
        2181
               0
MOTA
                                                                                   Н
                                                                1.00 32.05
                                                       40.387
                                              31.564
                                    123.473
                    THR
                            69
         2182
               N
 MOTA
                                                                                   н
                                                                 1.00 37.56
                                              30.874
                                                        40.429
                                    122.192
               CA
                    THR
                            .69
         2183
 MOTA.
                                                                                   Ή
                                                                \cdot 1.0035.94
                                              29.541
                                                       39.655
                                    122.284
                            69
               CB
         2184
                    THR
 MOTA
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                                                                 1.00 40.10
                                                        38.253
                                    122.392
                                              29.821
                            69
                    THR
               OG1
 MOTA
         2185
                                                                                   н
                                                                1.00 26.92
                                    121.065
                                                       39.908
                                              28.676
                            69
               CG2
                    THR
         2186
 MOTA
                                                                                   Н
                                                                 1.00 43.54
                                                       41.914
                                    121.915
                                              30.626
               С
                    THR
                            69
         2187
 MOTA
                                                                 1.00 40.52
                                                                                   H
                                                        42.550
                                              29.823
                                    122.595
                            69
               0
                    THR
         2188
 MOTA
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                                                                 1.00.45.97
                                                        42.469
                                    120.924
                                               31.319
                            70
               Ŋ
                    LEU
         2189
 MOTA.
                                                                                   н
                                                                 1.00 46.62
                                                        43.893
                                               31.189
                            70
                                    120.622
                CA
                    LEU
         2190
 MOTA
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                                                                 1.00 47.28
                                                        44.445
                                              32.536
                                    120.166
                    LEU
                            70
         2191
                CB
 MOTA
                                                                                   Н
                                                                 1.00 55.81
                                                        45.091
                                               33.331
                                    121.305
         2192
                CG
                    LEU
                             70
 ATOM
                                                                                   Н
                                                                 1.00 43.73
                                                       .44.767
                                               34.805
                             70
                                    121.133
         2193
                CD1
                    ·LEU
 MOTA
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                                                                 1.00 43.94
                                               33.094
                                                        46.611
                                    121.322
                            70
                CD2 LEU
 ATOM
         2194
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                                                                 1.00 43.94
                                                        44.312
                                              .30.107
                                    .119.636
                             70
                    LEÚ
         2195
                C
 MOTA
                                                                                   н
                                                                 1.00 42.32
                                                        43.849
                                               30.070
                                    118.496
                             70
                    LEU
         2196
                0
 ATOM
                                                                 1.00 44.21
                                                                                   H
                                                        45.218
                                               29.247
                                     120.103
                             71
         2197
                N
                     TLE
 ATOM
                                                                 1.00 49.89
                                                                                   н
                                                        45.755
                                               28.125
                                    119.333
                     ILE
                             71.
                CA
 MOTA
         2198
                                                                 1.00 51.60
                                                                                   Н
                                                        45.430
                                               26.770
                     ILE
                             71
                                     120.026
                CB ·
         2199
 MOTA
                                                                                   Н
                                                                 1.00 29.06
                                                        46.072
                                               25.616
                                     119.259
         2200
                CG2
                     ILE
                             71
 MOTA
                                                                                    н
                                                        43.911
                                                                 1.00 54.43
                                     120.107
                                               26.573
                             71
         2201
                CG1
                     ILE
 MOTA
                                                                                    H
                                                                 1.00 43.28
                                                        43.222
                                               27.402
                                     121.184
                    ILE
                             71
                CD1
 MOTA
         2202
                                                                                    н
                                                        47.278
                                                                 1.00 52.79
                                               28.255
                                     119.203
                             71
                     ILE
         2203
                C
 MOTA
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                                                                 1.00 62.18
                                               28.779
                                                        47.939
                                     120.103
                0
                     ILE
                             71
         2204
 ATOM
                                                                                    H
                                                                 1.00 50.92
                                                        47.830
                                               27.768
                                     118.093
                             72
         2205
                N
                     VAL
  MOTA
                                                                  1.00 52.77
                                                                                    H
                                                        49.269
                                               27.843
                                     117.837
                             72
                     VAL
         2206
                CA
  MOTA
                                                                  1.00 47.96
                                                                                    H
                                                        49.549
                                               28.677
                             72
                                     116.551
                     VAL
          2207
                CB
  ATOM
                                                                                    н
                                                                  1.00 44.08
                                               27.828
                                                         49.317
                                     115.313
                     VAL
                             72
         2208
                CGl
  ATOM ..
                                                                                    H
                                                                 1.00 43.63
                                                        .50.967
                                               29.224
                                     116.569
                             72
         2209
                CG2
                     VAL
  MOTA
                                                                                    н
                                                                  1.00 56.26
                                                        49.861
                                     117.687
                                               26.437
                     VAL
                             .72
                 C
  ATOM
          2210
                                                                                    H
                                                                  1.00 65.48
                                                         49.123
                                     117.627
                                               25.457
                             72
                     VAL
                 0 .
  MOTA
          2211
                                                                                    Н
                                                                  1.00 56.09
                                                         51.191
                                     117.638
                                                26.344
                     ASP
                             73
                 N
          2212
  MOTA
                                                                                    н
                                                                  1.00 50.35
                                     117.492
                                                25.064
                                                        51.891
                             73
                 CA
                     ASP
          2213
  MOTA
                                                                                    H
                                                                  1.00 53.65
                                                         51.995
                                     118.848
                                                24.365
                             73
                 CB
                     ASP
  MOTA
          2214
                                                                                    Н
                                                                  1.00 57.99
                                                         52.384
                                                22.907
                                     118.721
                              73
                 CG
                     ASP
          2215
  ATOM .
                                                                                     H
                                                                  1.00 57.92
                                                         53.443
                                                22.616
                                      118.119
                              73
                 OD1 ASP
          2216
  MOTA
                                                                  1.00 61.79
                                                                                     H
                                                         51.625
                                      119.229
                                                22.055
                 OD2
                     ASP
                              73
          2217
  MOTA
                                                                                     H
                                                                        50.51
                                                         53.290
                                                                  1.00
                                      116.932
                                                25.313
                              73
          2218
                 Ċ.
                      A:SP
  MOTA
                                                         54.280
                                                                  1.00
                                                25.288
                                      117.664
                 0
                      ASP
  ATOM
          2219
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•		•					53.352	1.00 56.54	H
MOTA	2220	N	THR	74		25.535	54.593	1.00 66.24	H .
MOTA	2221	CA	THR	74	114.913	25.836	54.296	1.00 71.27	H
ATOM	2222	CB	THR	.74		.26.020	52.901	1.00 71.81	н
ATOM	2223	OG1	THR	74	113.183	25.793	54.659	1.00 81.34	H
MOTA	2224	CG2	THR	74	112.979	27.430		1.00 71.66	H
ATOM	2225	C·	THR	74	115.054	24.876	55.785	1.00 67.59	. н
ATOM	2226	0	THR	74		25.220	56.902	1.00 37.35	H
ATOM	2227	N	SER	75	115.610	23.689	55.559	1.00 75.40	H
ATOM	2228	CA	SER	75		22.712	56.634	1.00 89.23	H
ATOM	2229	СВ	SER	75	115.833	21.292	56.063	1.00 75.33	н
ATOM	2230	OG	SER	75 .	116.615	20.445	56.891	1.00 60.40	. н
ATOM	2231	С	SER	75	117.024	22.961	57.474		н
MOTA	2232	0	SER	75	116.949	23.066	58.703	1.00 51.38	. н
ATOM	2233	N	SER	76	118.171		56.807	1.00.45.77	н
ATOM	2234	CA	SER	76	119.435	23.282	57.498	1.00 44.97	·H
ATOM	2235	CB	SER	76	120.585	22.601		1.00 51.28	H
ATOM	2236	OG	SER	76 ·	120.106	21.807	55.676	1.00 43.07	H .
ATOM	2237	C	SER	76 ·	119.691	24.781	57.589	1.00 34 83	H
ATOM	2238	o	SER	76	120.755	25.221	58.008	1.00 28.11	
	2239	N	ASN	77	118.697	25.563	57.194	1.00 46.96	H
MOTA	2240	CA	ASN	77	118.826	27.009	57.222	1.00 38.99	H
ATOM .	2241	CB	ASN	77	118.847	27.513	58.665	1.00 41.25	H
MOTA	2242	CG	ASN	77	117.459	27.785		1.00 39.52	H.
MOTA	2242		LASN	.77	.116.470	27.731	58.468	1.00 40.29	H
ATOM	2244		ASN	77	117.377	28.082	60.496	1.00 23.39	H
MOTA		C	ASN	77	120.111	27.395	56.515	1.00 34.49	H
MOTA	2245	0	ASN	77	120.971	28.067	57.077	1.00 45.69	н
MOTA	2246 2247	Ŋ	THR	78	120.240	26.944	55.275	1.00 39.07	H
ATOM	2247	CA	THR	78	121.417	27.244	54.481	1.00 43.99	H
ATOM		CB	THR	78	122.340	26.001	54.336	1.00 47.54	. Н
ATOM	2249		1 THR	78	121.955	25.239	53.189	1.00 23.72	. H
ATOM	2250 2251	CG		.78	122.244	25.122	55.568	1.00 19.39	H
ATOM	2252	C	THR	78	121.030	27.761	53.100	1.00 35.58	н
MOTA	2252		THR	78	120.107	27.255		1.00 41.21	·H
ATOM	2254		ALA	79	121.738	28.791		1.00 32.09	H
MOTA	2254			79	121.498		51.361		H
ATOM				79	121.265				H
MOTA	2256 2257		ALA	79 -	122.734				H
MOTA	2258		ALA	79	123.854	29.447			H
ATOM			TYR	80	122.550	28.589	49.321		. · H
ATOM	2260			80	123.697	28.329		1.00 32.51	H
MOTA	2261			•	123.635	26.921	47.920		н
MOTA	2262			80	123.465	25.846			H
ATOM	2263		1 TYR	80	124.539	25.04.9			'H.
MOTA	2264		1 TYR	80	124.37				H
MOTA	2265		2 TYR	. 80	122.212	2 25.575			Н
ATOM	2266		E2 TYR	80	122.028	3 24.529			H
ATOM				80	123.11		2 50.759		H
MOTA						3 22.69			H
MOTA			·TYR	80	123.81		7 47.32		Н
MOTA			TYR	_	122.87	0 30.01		1 1.00 54.32	H
MOTA			MET	81	125.01	2 29.32			н
ATOM				81	125.34		5 45.60		H
ATOM	241				•				

	•							. 00 47 13	H
ATOM	2273	CB	MET	. 81	126.117	31.401	46.073 45.151	1.00 47.13 1.00 49.47	H
MOTA	2274	CG	MET	81	127.250	33.310	44.268	1.00 52.80	H
ATOM	2275	SD	MET	81	126.890	34.508	45.421	1.00 52.92	н
MOTA	2276	CE:	MET	81	127.508		44.699	1.00 51.47	H
MOTA	2277	C	MET	81	126.220	29.327	45.065	1.00 48.72	н
MOTA	2278	0	MET	81 .	127.342	28.976	43.525	1.00 46.87	н
MOTA	2279	N	GLN	82	125.707	28.981	42.595	1.00 45.38	H
MOTA	2280	CA	GLN	82	126.476	28.175	41.943	1.00 71.53	н
MOTA	2281	CB	GTN	82	125.589	27.113	40.511	1.00 89.74	н
MOTA	2282	CG	GLN	82	125.978	26.739	40.433	1.00 96.73	Н
MOTA	2283	CD	GLN	82	127.278	25.955 25.699	41.448	1.00 98.73	н
MOTA	2284		GLN	82	127.925 127.665	25.572	39.220	1.00 94.58	H
MOTA	2285	NE2		82		29.065	41.530	1.00 44.59	H
MOTA	2286	Ċ	GLN	82	127.075	29.787	40.833	1.00 42.20	н
MOTA	2287	Ò	GľN	82	126.366	29.767		1.00 49.17	н
MOTA	2288	N	LEU	83	128.394	29.014	40.434	1.00 46.27	н
MOTA	2289	CA	LEU	. 83	,	30.398	41.067	1.00 32.33	Η.
MOTA	2290	CB	LEU	83	130.369	31.416	42.160	1.00 31.17	H
Moța	2291	CG	LEU	. 83	130.033	31.455	43.252	1.00 6.90	H.
MOTA	2292		LEU	. 83	131.119 129.865	32.766		1.00.18.19	H.
MOTA .	2293		LEU	83	129.865	28.845	39.298	1.00 45.11	н
MOTA	2294		LEU	83	130.201	27.870	39.496	1.00 36.84	H
MOTA	2295	0	LEU	83	128.925	29.118	38.117	1.00 44.08	H
MOTA	2296	N	SER		129.160	28.280	36.948	1.00 46.97	H
MOTA	2297	CA	SER	84	127.829	27.869	36.323	1.00 54.37	H
MOTA	2298	CB	SER		127.604	28.576	35.118	1.00 64.19	H
MOTA	2299	OG	SER	84	130.037	28.942	35.896	1.00 49.55	H
ATOM	2300	C	SER	84	129.905	30.137	35.617	1.00 47.92	H
MOTA	2301	•	SER	84	130.925	28.146	35.306	1.00 48.23	H
MOTA	2302	N	ARG	85 85	131.842	28.637	34.294	1.00 41.86	H
MOTA	2303	CA	ARG	· 85	131.042	29.141	33.082	1.00 46.21	H
MOTA	23.04	CB	ARG ARG	85	130.474	28.012	32.236	1.00 41.59	H
ATOM	2305	CG	ARG	85	129.125		31.630	1.00 68.47	H.
MOTA	2306		ARG	85	129.174	28.406	30.170	1.00 68.50	H
MOTA	2307	NE CZ	ARG	85	128.142		29.381	1.00 60.66	H.
MOTA	2308		L ARG	85	126.962	27.808	29.906	1.00 56.39	H
MOTA	2309		ARG	85	128.293	28.166	28.065	1.00 55.47	· H
MOTA	2310		ARG	85	132.670	29.752	34.912	1.00 40.27	. н
ATOM	2311	С 0	ARG	85	132.430	30.939	34.669	1.00 37.17	н
MOTA	2312	И	MET		133.645	29.350	35.722	1.00 35.41	H
MOTA	2313 2314	CA		86	134.518	30.288	36.412	1.00 32.72	H
MOTA			MET	. 86	134.974	29.684	37.733	1.00 38.34	. н
MOTA	2315 2316		MET	86	134.091	28.551	38.215	1.00 45.32	H
ATOM	2317		MET	86	133.310	28.856	39.804	1.00 63.97	н
MOTA	2317		MET	86	133.680	30.599	40.068	1.00.45.50.	
MOTA	2319		MET	86	135.733	30.691	35.592	1.00 33.88	H
ATOM	2320	_	MET	. 86	136.097	30.018	. 34.627	1.00 28.01	H
ATOM	2320		THR	87	136.357	31.794	35.996	1.00 37.82	H
MOTA	2322			87	137.525	32.330			
MOTA MOTA	2323			87	137.081		34.035		H
MOTA			1 THR	87	136.455		33.153		
MOTA	2325		2 THR	87	138.263		33.324	1.00 41.18	н
WION				•			• .		•

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1.00 49.08
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                                               33.282
                                   138.299
                            87
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                                                        37.278
                                   . 137.797
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ATOM	2436	CD1	TYR <sup>.</sup>	101	110.933	39.404	51.945	1.00 27.58	н
ATOM	2437	CEl	TYR	101	110.024	39.324	50.885	1.00 27.56	H
ATOM	2438	CD2	TYR	101	109.135	39.502	53.507	1.00 40.43	н
ATOM	2439	CE2	TYR	101	108.216	39.422	52.450	1.00 40.43	H
ATOM	2440	CZ	TYR	101	108.673		51.145	1.00 27.74	н
ATOM	2441	OH	TYR .	101	107.779	39.275	50.100	1.00 40.21	H
ATOM	2442	С	TYR	101	111.167	41.950	55.247	1.00 33.30	H
MOTA	2443	Ο.	TYR	101	111.013		56.470	1.00 45.70	н
ATOM	2444	N	GLY	102	110.525			1.00 43.70	н
ATOM	2445	CA	GLY	102 .	109.611		55.079	1.00 43.01	н.
	2446	C	GLY .	102	110.364		55.237	1.00 47.90	н
ATOM	2447	0	GLY	102	110.169		54.464	1.00 47.30	H
ATOM	2448	N	LEU	103	111.229		56.243	1.00 34.98	H
ATOM	2449	CA	LEU.	, 103	112.062		56.475	1.00 47.24	. н
ATOM	2450	CB	LEU	103	.112.270		57.975	1.00 47.24	·H
MOTA	2451	CG	LEU	103	111.258		58.750	1.00 30.12	н
MOTA	2452	CD1	LEU	103	109.959		57.956	1.00 44.52	H.
ATOM	2453	CD2	LEU	103	110.993		60.092	1.00 31.85	. н
ATOM	2454	С	LEU	103	113.394		55.807	1.00 32.76	. н
ATOM	2455	0	LEU .	103	114.392	<b>-</b>	56.471	1.00 33.42	H
ATOM	2456	. N	ASP	104	113.368		54.477		н
ATOM	2457	CA	ASP	104	114.512		53.625	1.00 32.02	н
ATOM	2458	CB	ASP	104	113.997		52.295	1.00 55.62	. H
MOTA	2459	CG	ASP	104	115.09		51.298 50.136	1.00 38.63	н
MOTA	2460	OD1	ASP	104	114.75		51.663	1.00 61.09	H
ATOM	2461	OD2	ASP	104	116.28		53.415	1.00 29.02	H
ATOM	2462	C.		104	115.25		52.440	1.00 33.69	. н
ATOM	2463	. O	ASP	104	115.02		54.346	1.00 37.55	H
ATOM	2464	Ņ	TRP	105	116.14		54.288	1.00 32.28	н
MOTA	2465	CA	TRP	105	116.90		55.518	1.00.42.44	н
MOTA	2466	CB	TRP	. 105	116.59	_	55.717	1.00 44.69	H
ATOM	2467	CG	TRP	105	115.12			1.00 43.59	н
MOTA	2468		TRP	105	114.45 113.09				н
MOTA	2469	CE		105	114.88	·			H
MOTA	2470	CE:		105	114.35	•			H
MOTA	. 2471				112.94				Н
ATOM	2472	NE:		105	112.14				н
MOTA	2473			105	113.94			,	· H
MOTA	. 2474			105	112.58				. н
MOTA	2475		2 TRP	105	118.40			·	H
MOTA	2476		TRP		119.06				H
MOTA	2477		TRP	105	118.99				H
MOTA	2478		•		120.38			1.00 46.39	H
MOTA					120.30				H
MOTA				•	120.86				H
MOTA					119.90			3 1.00 32.97	
MOTA			1 ASN		121.7			1.00 41.71	H
MOTA			2 ASN		120.7				H
MOTA	2484	Ł C	ASN	. 106	2200	•			_

						•		1 00 46 93	Ħ
ATOM	2485	0	ASN	106	119.950		55.760	1.00 46.92 1.00 47.37	H
ATOM	2486	N	PHE	107 ·	122.079		55.202	1.00 47.06	н
ATOM	2487	CA	PHE	107	122.665		55.489	1.00 47.00	. н
MOTA	2488	CB	PHE	107	123.589		54.341	1.00 36.58	н
ATOM	2489	CG	PHE .	107 .	123.004		52.954	1.00 43.99	H.
MOTA	2490	CD1	PHE .	107	121.628		52.737	1.00 45.33	H
ATOM	2491	CD2	PHE	107	123.847		51.851	1.00 35.20	H
ATOM	2492	CEl	PHE	107	121.107		51.449	1.00 20.31	н
ATOM	2493	CE2	PHE	107 ·	123.334		50.561	1.00 20.31	н
ATOM	2494	cz	PHE	107	. 121.965		50.362	1.00 45.87	• н
ATOM	2495	C	PHE	107	123.479	44.386	56.787	1.00 38.80	н
MOTA	2496	0	PHE .	107	124.641	44.805	56.765	1.00 44.31	H
ATOM .	2497	N	ASP	108	122.874	43.982	57.905	1.00 44.31	H
ATOM	2498	CA	ASP	108	123.528	44.053	59.215	1.00 40.40	н
ATOM	2499	CB	ASP	108	122.479	44.243	60.325	1.00 66.26	н
ATOM	2500	CG	ASP	108	121.048	44.057	59.833	1.00 56.03	н
ATOM	2501	OD1	ASP	108	120.304	45.059	59.790	1.00 63.18	н
MOTA	2502		ASP	108	120.664	42.914	59.494	1.00 63.13	H
ATOM	2503	C	ASP	108	124.445	42.889	59.600	1.00 27.33	н
MOTA	2504	0	ASP	108	125.418	43.077	60.328	1.00 18.58	н
ATOM	2505	N.	VAL	109	124.133	41.690	59.128	1.00 20.11	н
ATOM	2506	CA	VAL	109	124.946	40.527	59.458	1.00 25.57	H
ATOM	2507	CB	VAL	109	124,072	39.410	60.037	1.00 23.37	н
MOTA	2508	CG1	VAL	109	124.936	38.353	60.691	1.00 21.93	н
ATOM	. 2509	. CG2	VAL	109	123.098	39.998	61.038		H
MOTA	2510	C.	VAL	1.09 ·	125.704	39.984		1.00 28.04	H
ATOM	.2511	0	VAL	109	125.110	39.594	57.248	1.00 34.75	H
ATOM	2512	И	TRP	110	127.023	39.949	58.336	1.00 27.30	H
ATOM	, 2513	CA	TRP	110	127.818	39.459	57.229	1.00 27.20	. н
ATOM	2514	CB	TRP	110	128.834	40.519	56.810	1.00 35.70	н
ATOM	2515	CG	TRP	110	128.248	41.738	56.167	1.00 25.48	. н
MOTA	2516	CD2	TRP	110	128.440	42.162	54.813 54.669	1.00 33.24	н
MOTA	2517	CE:	2 TRP	110	127.801	43.411	53.711	1.00 13.14	н
ATOM	2518	CE:	3 TRP	110	.129.097	41.609	56.770	1.00 42.55	,H
ATOM	2519	CD:	1 TRP	110	127.511		55.879		H
ATOM	2520	NE:	1 TRP	110	127.236		53.467		н
ATOM	2521	CZ	2 TRP	110	. 127.795		52.511		H
MOTA	2522	CZ	3 TRP.	110 ·	129.096		52.402		H
MOTA	2523	CH	2 TRP	110	128.449		57.601		н
MOTA	2524	C	TRP	110	128.566		58.753		н
MOTA	. 2525	0	TRP	110	128.946		.56.621		. н
MOTA	2526	· N	GLY	111	128.774				H
ATOM	2527	CA CA		111	129.523		56.847	•	H
MOTA	2528	C	GLY	111	130.988				H
ATOM	2529	9 0	GLY	. 111	131.327				. Н
MOTA	2530	N	ALA	112	131.867				H
MOTA	2531	L CA		. 112	133.287				H
ATOM		2 CE		112	134.033				н
ATOM	•	3 C	ALA	112	133.857	7 35.896 2 36.492		1.00 49.85	н
MOTA		4 0	ALA	112	134.90				н
MOTA		5 N	GLY	113	133.17				Ħ
ATOM	253			113	133.66				H
MOTA	253	7 C,	GLY	113	134.18			· · .	

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53.894
                                                                1.00
                                                                     40.99
                                                                                  H
                                   134.273
                                             32.862
                   GLY
                          113
       2538
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MOTA
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                                                                1.00
                                                                     44.31
                                   134.519 33.690
                                                      51.819
              N
                   THR
                          114
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MOTA
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                                                      51.242
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                                             32.446
                          114
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ATOM
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ATOM
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MOTA
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MOTA
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                                                                1.00 42.98
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MOTA
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                                                                1.00 36.59
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MOTA
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                                                                1.00 42.28
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                                                       39.060
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                                                        38.919
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 MOTA
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                                                        39.445
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 ATOM
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                                                        40.432
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 MOTA
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1.00 48.35
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MOTA
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ATOM
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MOTA
        2605
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MOTA
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MOTA
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ATOM
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 MOTA
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                           124
        2611
               CG2
                   THR
ATOM
                                                                                  H
                                                                1.00 61.90
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                                                       48.776
                                    152.034
        2612
               C
                    THR
                           124
 MOTA
                                                                                  н
                                              24.005
                                                                1.00 66.47
                                                       49.113
                                    151.832
                    THR
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MOTA.
        2613
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                                              21.918
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                    PRO
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 MOTA
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                                                                1.00 60.12
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               C
                    PRO
                           125
 MOTA
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                                                       50.329
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                    PRO
                           125
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 MOTA
        2620
                                                                1.00 55.19
                                                                                   H
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                                             24.153
                                                       52.140
                    PRO
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· ATOM
        2621
               N
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                                                       53.169
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                    PRO
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 MOTA
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               CD
                                                                1.00 47.53
                                                                                  ·H
                                              25.156
                                                       52.333
                                    154,855
                           126
                    PRO
               CA
 ATOM
         2623
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                                                                 1.00 49.84
                                              26.141
                                                       53.296
                                    154.213
                    PRO
                           126
               CB
         2624
 ATOM
                                                                                   H
                                                                 1.00 73.92
                                                       54.118
                                    153.315
                                              25.289
         2625
               CG
                    PRO
                           126
 MOTA
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                                                                 1.00 49.11
                                              24.608
                                                       52.891
                                    156.155
               C
                    PRO
                           126
         2626
 MOTA
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                                                                 1.00 53.71
                                                       53.716
                                    156.148
                                              23.695
                           126
               O.
                    PRO
         2627
 MOTA
                                                                                   н
                                                        52.429
                                                                 1.00 38.85
                                              25.174
                                    157.266
               N
                    SER
                           127
         2628
 MOTA
                                                                                   Н
                                                                 1.00 21.97
                                                        52.913
                                              24.792
                                    158.586
         2629
                    SER
                           127
               ÇA
 MOTA
                                                                                   Н
                                                                 1.00 39.50
                                                        51.798
                                              24.904
                                    159.628
               CB
                           127
         2630
                    SER
 ATOM
                                                                                   H
                                                                1.00 52.42
                                                        50.845
                                              23.866
                                    159.487
                           127
                    SER
                OG
 MOTA
         2631
                                                                                   H
                                                                 1.00 33.98
                                                       53.990
                                               25.826
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                           127
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                C
         2632
 ATOM
                                                                                   Н
                                                                 1.00 34.88
                                               27.008
                                                        53.687
                                    159.021
                0
                     SER
                           127
         2633
 MOTA
                                                                                   H
                                                                 1.00 39.20
                                                        55.243
                                    158.903
                                               25.393
                     VAL
                           128
                N
         2634
 MOTA
                                                                                   Н
                                                                1.00 46.26
                                                        56.353
                                               26.308
                                    159.135
                    VAL
                           128
         2635
                CA
 MOTA
                                                                                   H
                                                        57.562
                                                                 1.00 49.37.
                                               25.929
                                     158.247
         2636
                CB
                     VAL
                           128
 MOTA
                                                                                   H
                                                                 1.00 42.90
                                                        58,545
                                               27.089
                                     158.162
                CG1
                    VAL
                            128
         2637
 MOTA
                                                                                   H
                                                                 1.00 51.53
                                                        57.078
                                     156.862
                                               25.538
                            128
         2638
                CG2
                    VAL
 MOTA
                                                                                   H
                                     160.594 26.350
                                                                 1.00 37.55
                                                        56.794
                     VAL
                            128
                C
 ATOM
         2639
                                                                                    H
                                                                 1.00 49.56
                                               25.329
                                                       .57.153
                                     161.183
                     VAL
                            128
         2640
                0
 ATOM
                                                                                    н
                                     161.172 27.545
                                                        56.765
                                                                 1.00 48.51
                     TYR
                            129
         2641
                И
 MOTA
                                                                                    Н
                                                                 1.00 44.86
                                     162.562
                                               27.740
                                                        57.150
                            129
                CA
                     TYR
         2642
 MOTA
                                                                  1.00 35.54
                                                                                    H
                                                        55.969
                                               28.279
                                     163.364
                     TYR
                            129
                CB
  MOTA
          2643
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	•	• •	• • • • • •		163.348 27.402 54.736 1.00 27.55 H
MOTA			TYR	129	163.310 26.059 54.800 1.00 42.44 H
ATOM	2645		TYR	129	163.718 26.059 54.800 1.00 42.44 H
MOTA	2646		TYR	129	103.725 25.22
MOTA	.2647		TYR	129	102.300 H
MOTA	2648		TYR	129	102.331 H
MOTA	2649	_	TYR ·	129	100.000
ATOM .	2650	ОН	TYR ·	129	103.300
MOTA	2651	C .	TYR	129	102,070
ATOM .	2652	0	TYR '	129	102.10
ATOM	2653	N	PRO	130	103,300
MOTA	2654	CD .	PRO '	130	H
MOTA	2655	CA	PRO	130	163.482 29.152 00.25, 2.0
ATOM	2656.	CB.	PRO.	130 .	163.970 28.180 01.002 2.00 50 96 H
ATOM	2657	CG	PRO	130	164.699 .27.132 80.872 1.00 20.42 13 H
MOTA	2658	G.	PRO	130	164.486 30.276 60.333 2.00
ATOM	2659	.0	PRO	130	165.506 30.079 35.702 2.00 40 93
ATOM	. 2660	$\mathbf{N}$ .	LEU .	131 .	TO U
MOTA	.2661	·CA .	LEU "	·131 . `	165.081 32.598 60.732 3.00
ATOM	2662	СB	LEU .	, 131 .	164.319 33.772 60.120 1.00
ATOM	2663	CG	_LEU	131	163.916 33.644 30.032
ATOM	2664		FEA	131 ·	163.135 34.878 58.245 1.00 25 67 H
ATOM'	2665	CD2	LEU	131	165,144 33.463 37.761 2.66
MOTA	2666	C.	LEU	131	165.666 33.014 .02.07 .1 00 46 95 H
MOTA	2667	٠٥.	LEU	.131	164.956 33.337 02.327 = 100.56.70 H
ATOM	2668	N·	ALA .	132	160.550 541.55
MOTA.	2669	CA	ALA .	132	167.632 33.110 63.307 1.00 57 53 H
MOTA	2670	CB	ALA.	132	168.300 31.888 64.036 1.00 5F.07 H
MOTA	2671	C	ALA	132	168.662 34.210 03.200 1.00 54.54
MOTA	2672	0	ALA	132	169.276 34.279 62.204 1.00
· ATOM	2673	N	PRO	133	168.864 35.091 64.202
ATOM	2674	CD	PRO	133	168.161 35.065 65.557 1.00 60 60 H
ATOM	2675	CA	. PRO	133	169.815 36.206 04.107 2.00
ATOM	2676	CB	PRO	133	169.496 37.030 03.434 200 46 95 H
ATOM	2677	CG.	PRO	133	168.946 36.033 66.333 1.00 20 64 47
ATOM	2678	, 'C	PRO	133	171.285 35.780 64.154 1.00 62.83
ATOM	2679	٠. О	PRO	133	171.743 35.030 65.021
ATOM	2680	N	GLY	134	172.021 36.276 63.101 1.00 54 50 H
ATOM	2681	CA	GLY.	134	173.429 35.937 63.030 1.00 50.13 · H
MOTA	2682	C	. GLY	134	174.356 36.531 64.074 1.00 70 75
MOTA	. 2683	ο.	GLY		175.515 BOOK 1 00 74 93
ATOM	2684	N .	SER	135	173.893 30.052 05.270 1.00 06 16 H
ATOM	. 2685	CA		135	174.743 37.218 88.319 1.00 00 22
ATOM	2686	CB	SER	135	170.000 T
ATOM.	2687		SER	135	176.965 36.773 03.225 - 00.00 57
ATOM	2688	· c	SER	135	175.096. 38.660 65.950 1.00 55.55
ATOM	2689	0	SER	135	176.088 38.320 33.23
MOTA	.,2690		ALA	136	174.255 39.332 CO. 15 W
MOTA	2691		ALA	136	174.413.40.992 88.208 1.00 90.25 H
ATOM	2692		ALA	136	174.299 41.304 04.714 1.00 02.00 H
ATOM	2693		ALA	136	173.334 41.739 00.302 1.00
ATOM	2694		ALA	136	172.158 41.398 00.310 1.00 00 00
ATOM	2695		ALA	137	173.740 42.610 07.633
ATOM	2696		ALA	137	172.802 43.637 88.417 1.002000
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	•	· .			173.565	44.631	69.285	1.00 89.73	н.
MOTA	2697		ALA	137	173.363		67.474	1.00.99.97	H
ATOM	2698	C	ALA .	137	172.119		67.094	1.00 99.95	H
MOTA	2699	0	ALA	137	•		67.103	1.00 99.99	H
MOTA	2700	N	GLN	138	170.768		66.198	1.00 99.99	H
MOTA	2701	CA	GLN	138	169.788		65.804	1.00 92.32	H
MOTA	2702	CB	GLN .	138	168,740.		66.972	1.00 80.27	·H
MOTA	2703	CG	GLN	138	167.946	42.702	66.679	1.00 62.10	H
MOTA	2704	CD		. 138	166.461	42.463	65.530	1.00 72.23	H
MOTA	2705	OE1		138	166.051	42.749	67.720	1.00 47.02	H
ATOM	2706	NE2	GLN	138	165.646	45.522	66.818	1.00 99.97	H
MOTA	2707	C	GLN	138	169.100	46.516	66.136	1.00 99.97	H
MOTA	2708	Ο.	GLN	138	168.850	45.438	68.116	1.00 99.99	H
ATOM	2709	N	THR	139	168.797	46.530	68.810	1.00100.00	H
MOTA	2710	CA	THR	139	168.138	46.520	68.570	1.00100.00	,H
ATOM	2711	CB	THR	139	166.629	45.306		1.00 99.99	H
ATOM	2712	OG1		139	166.068	45.506	67.084	1.00 99.99	H
MOTA	2713	CG2	THR	. 139	166.326		70.301	1.00 99.99	. <b>H</b>
MOTA	2714	C	THR	139	168.421	46.461	71.014	1.00 99.98	н
MOTA	2715	0	THR	139	167.865	45.622	70.792		H
MOTA	2716	N	ASN.	140	169.282	47.359	72.187	1.00 96.92	H
MOTA	2717	CA	ASN	140	169.654	47.435	72.927	1.00 94.82	H
ATOM	2718	CB	asn	140	168.714	48.381	72.357		H
ATOM .	2719	ĊĠ	ASN .	140	168.783	49.786		1.00 88.37	н
MOTA	2720	QD1	ASN	140	169.866		.72.032	1.00 91.05	н
ATOM	2721	ND2	ASN	140	167.633		72.229	1.00 93.43	. н
MOTA	2722	C	ASN	140	169.724	46.052	72.801	1.00 83.04	H
ATOM	2723	0	ASN	140	170.715	45.321	72.647	1.00 91.74	н
ATOM	2724	N	SER	141	168.684	45.691	73.529	1.00 78.99	· H
MOTA	2725	CA	SER	141	168.629	44.391	74.200 75.629	1.00 70.33	H
MOTA	2726	CB	SER	141	168.101	44.544	75.629	1.00 60.50	н
ATOM	2727	OG	SER	141	166.899	45.297	73.432	1.00 75.37	H
ATOM	2728	C	SER	141	167.726	43.431	72.896	1.00 88.08	Н
ATOM	2729	0	ŞER	141	168.173	42.413	73.391	1.00 59.56	·H
MOTA	2730	N	MET	142	166.479	43.787		1.00 44.97	н
ATOM	2731	CA	MET	14.2	165.449		72.766 72.516		н
MOTA	2732	CB	MET	142	164.206		73.800	1.00 86.09	н
ATOM	2733	CG	MET	142	163.645		73.535		н
MOTA	2734	SD	MET	142	162.177		74.546	1.00 99.42	Н
ATOM	2735	CE	MET	. 142	162.239		71.432	1.00 32.94	H
ATOM	2736	. C.	MET	. 142	165.871		70.772	1.00 33.63	. H
MOTA	2737	0	MET	142	166.780		71.027		. )H
MOTA	2738		VAĹ	143	165.183		6.9.779	1.00 24.76	H
ATOM	2739	CA	· VAL	143	165.501		70.065		. н
MOTA	2740			143	166.197			1.00 34.15	H
ATOM	2741		1 VAL	143	165.186				н
MOTA	2742		2 VAL	143	166.872				н
ATOM	2743		VAL	143	164.299				, H
ATOM	2744		VAL	143	163.150				н
ATOM	2745	N	THR	. 144	164.588	39,981			н
ATOM			THR	144	163.56				н
ATOM	2747		THR	144	163.45				н
ATOM	2748	_	1 THR	144	162.934	41.991			H
ATOM			2 THR	144	162.54	3 40.394	64.436	, 1.00 20.05	
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	·	•	•				00 204	65.891	1.00 3	9.99	· H	
MOTA	2750	C,	THR	144	163.		38.384 38.178	65.384	1.00 4		H	
MOTA	2751	0	THR	144	164.		37.507	65.830	1.00		н	
MOTA	2752	Ŋ	LEU	145	162.		36.237	65.138	1.00		н	
MOTA	2753	CA	LEU	145	163.		35.082	66.062	1.00		H,	
ATOM	2754	CB	LEU	145	162.			67.003	1.00		н	
ATOM	2755	CG	LEU	145	163.		34.615	68.376	1.00		H.	
ATOM	2756		LEU	145	163.		35:237		1.00		· н	
ATOM	2757	CD2	LEU	145	163.	•	33.095	67.084	1.00		н	
MOTA	2758	C ·	LEU	145	162:		36.220	63.948	1.00		н	
MOTA	2759	0	LEU	145	161.		37.073	63.831	1.00		н	
ATOM	2760	N	GLY	146	162.		35.240	63.072	1.00		н	
ATOM	2761	CA	GLY	146	161.		35.153	61.903			H	
ATOM	2762	C	GLY	146	161.		33.741	61.381		19.61	H	
ATOM	2763	0	GLY	146	.161.		32.845				H	
ATOM	2764	N	CYS	147	160.	283	33.553	60.499		39.08	н	
ATOM	2765	CA	CYS	147	160.			59.885		38.87	. н	
	2766	C	CYS	147	159.	696	32.518	58.425		30.42	H	
MOTA	2767		CYS	147	158	934	33.431	58.109		37.75		
MOTA	2768	CB	CYS	147	158		31.560	60.574		55.35	H	
MOTA	2769	SG	CYS	147	159	313	30.021	61.435		81.70	H	
ATOM		N:		148	160	. 288	31.730	57.536		28.82	H	
ATOM	2770	CA	LEU	148	160	.037	31.891	56.115		27.56	. H	
MOTA	2771	CB	LEU.	148		.363	31.967	55.352		34.75		i.
MOTA	2772	CG	LEU	148		.254	32.129	53.831		34.95		1
ATOM	2773		LEU	148	160	.549	33.425	53.488	1.00	18.93		H ,
ATOM	2774			148		. 636	32.111	53:219		21,.69		H
MOTA	2775	CD2	LEU	148		.187	30.737			24.86		H .
MOTA	2776	C.	LEO .			.576	29.572	55.663		30.70		н .
ATOM	2777	0	VAL	149	158		31.077	55.045		27.57		H
MOTA	2778	N		149		.091	30.096		1.00	25.23		H
MOTA	2779	CA	VAL VAL	149		.658	30.376		1.00	3.47		H
MOTA	2780	CB		149		.800	29.127			25.66		H
MOTA	2781			149		.695	30.830		1.00	15.58	•	H
MOTA	2782			149		.152	30.207			43.19		H
ATOM	2783		VAL	149		.520	31.080		1.00	55.54	,	H
MOTA	2784		VAL			.906	29.313		1.00	45.51		H
MOTA	2785		LYS	150		3.078	29.377			36.67		H
MOTA	2786			150		9.572	29.376		1.00	23.27		H
MOTA	2787			150		9.950	30.226	. 49.36		37.80		H
MOTA	2788	_		150		1.441	30.145			45.44		H
ATOM	2789			150		1.689	29.729		1.00	47.90		H
MOTA	2790			150		3.035	30.147	7 47.14	9. 1.00	74.67		H
MOTA	2791			.150			28.322			47.62		H
MOTA	2792		LYS	150		7.393	27.22			61.91		Н
MOTA	2793	3 0	LYS	150		7.086	28.68			52.19		H
MOTA	2794	ı N	GLY	151	15	7.172			_	56.42	•	H
MOTA	2795			1:51		6.562				65.95		H
MOTA	2796		GLY	151	15	5.344				83.19		H.
MOTA	279	7 0	GLY	151	. 15	5.404				0 68.59		H
MOTA.		8 N	TYR		. 15	4.238				0 57.51		H
MOTA	279	9 C2		152			26.91 27.13			0 55.56		H
ATOM						2.646	•			0 49.75	•	H
ATOM						2.211				0 37.14		H
ATOM		2 C	D1 TYR	152	15	0.893		5 50.35				

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30.222
                                                        50.847
                                                                 1.00 37.53
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                                    150.474
                    TYR
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         2803
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                                                        51.250
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                    TYR
                           152
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ATOM
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                           152
                                    152.696
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                                                        51.605
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                    TYR
ATOM
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                                                                                    н
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               CZ
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                                    151.379
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ATOM
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                    TYR
ATOM
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ATOM
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                                               26.567
ATOM
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ATOM
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                    PHE
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                                                                                    H
                    PHE
                           153
                                    150.003
MOTA ·
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                                                        44.725
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                                                                 1.00 66.83
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                                    148.786
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                                                        44.147
 MOTA
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                                                                                    Н
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                           153
ATOM
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         2819
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                                                                                    Ή
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               N
                    PRO
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                                                        47.815
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                                                                                    H
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         2822
 MOTA
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                           154
                                     146.931
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                                                                 1.00 44.22
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 ATOM
                                                                                    Н
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                                                        46.772
                                                                 1.00 48.46
 MOTA
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                                                                                    H
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                                     144.923
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 ATOM
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                                                                 1.00 48.75
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                                                        49.722
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                                                        49.927
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                                                                                    H
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 ATOM
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 MOTA
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                                                        49.519
                                                                  1.00 52.55
 ATOM
         2831
                CG
                    GLU.
                                                                  1.00 54.96
                                                                                    H
                                     147.866
                                               33.696
                                                        50.773
 MOTA
         2832
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                                                32.945
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ATOM	2909	Ο,	SER	165		152.276	33.809	73.989	1.00 41.0		F	
ATOM	2910	N	LEU	166		152.385	33.049	71.883	1.00 56.74		F	
MOTA	2911	CA	LEU	166		153.102	34.227	71.421	1.00 37.44			H
MOTA	2912	CB	LEU	166		154.493	33.841	70.923				H
MOTA	2913	CG	LEU	166 .		155.626	34.088	71.922	1.00 41.75			H
MOTA	2914	CD1	LEU	-166		156.948	33.782	71.254	1.00 36.73			H.
MOTA	2915	CD2	LEU	166		155.598	35.532	72.416	1.00 58.4			H
ATOM	2916	С	LEU	166		152.318	34.920	70.319	1.00 60.23			H
	2917	0	LEU	166 ;		152.399	34.547	69.147	1.00 63.0			H
ATOM	2918	N	SER	167		151.547	35.928	70.708	1.00 65.9			H
ATOM	2919 ·	CA	SER	167	٠	150.740	36.684	69.762	1.00 64.7			H
ATOM	2920	CB	SER	167		149.255	36.347	69.946	1.00 66.6			H
MOTA	2921	OG	SER	167		148.697	37.030	71.057	1.00 54.2			H.
MOTA	2922	С	SER.	167	٠.	150.978	38.172	69.977	1.00 65.4		-	H.
MOTA	2923	0	SER	167		150.141	39.009	69.637	1.00 63.9			H
MOTA	2924	N·	SER	168	• •	152.134	38.486		1.00 72.2			H
ATOM	2925	CA	SER	168		152.515	39.868	70.814	1.00 66.9			H.
ATOM	2926	ĊВ	SER	168		152.814	40.052		1.00 83.1			H
MOTA	2927	OG	SER	168		153.476	41.282	72.551	1.00 92.9			н
ATOM	2928	С	SER	168		153.754	40.212	69:997	1.00 58.0			H.
MOTA	2929	O	SER	168		154.694		69.922	1.00 58.0			H.
ATOM	2930.	N	GLY	169		153.754	41.392	69.381	1.00 49.6			H
ATOM	2931	CA	GLY	169	•	154.897		68.582				н
ATOM	2932	c·	GLY	169		155.088	40.916	67.366	1.00 44.0			н
ATOM	2933	0	GĽY	169		156.205	40.731	66.887	1.00 49.3			H
MOTA	2934	N	VAL	170		153.991	40.366	66,862	1.00 45.7			H .
ATOM	2935	CA.	VAL	170		154.058	39.506	65.697	1.00 34.3			H
MOTA	2936	CB	VAL	170	•	153.135	38.291	65.854	1.00 23.7			H
MOTA	2937	CG1	VAL	170		153.213	37.418	64.614	1.00 23.4			H
MOTA	2938	· CG2	VAL	170	٠	153.539	37.492	67.079	1.00 30.			H
MOTA	2939	C.	VAL	170 ·	•	153.660	40.269	64.445	1.00 37.7			н
ATOM	. 2940	Ο.	VAL	170		152.732	41.074	64.460	1.00 38.0			H '
ATOM	2941	N	HIS	171		154.383		63.364	1.00 33.0			H
ATOM	2942	CA	HIS	171		154.118	40.664	62.088 61.802				H
ATOM	2943	CB	HIS	. 171		155.167	41.743	62.636	·			Н
MOTA	2944	CG	HIS	171		155.011	42.971	62.783				H
MOTA	2945		2 HIS	171		155.806	44.055					H
ATOM	2946		1 HIS	171		153.923	43.182					H
MOTA	2947		1 HIS	171		154.053	44.343 44.896					·H
MOTA	. 2948		2 HIS	171		155.189						H
ATOM	2949	C	HIS			154.172						H
ATOM.	2950	. 0	HIS			155.251	39.250		_			H
MOTA	2951			172		153.012			1.00 37			H
MOTA	2952			172		152.974				37		H
MOTA	2953			172		151.865						H
MOTA	2954		1 THR	172		152.160						H
MOTA	2955			172		151.760						H
MOTA	2956		THR	172		152.708 151.690		•				H.
ATOM	2957		THR	172		153.635						H
ATOM	2958		PHE	173		.153.635						H
ATOM	2959			173	•	154.889						H
MOTA	2960			173		155.707						H
MOTA	2961	, CG	PHE	173		100.707						

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ATOM	2962	CD1	PHE	173	155.577	42.326	56.264	1.00	69.14	1	н
MOTA	2963	CD2	PHE	173	156.555	40.360	57.216	1.00	71.48	. 1	H
ATOM	2964	CE1	PHE	173	156.277	43.117	57.165	1.00	47.16	!	H
ATOM	2965	CE3	PHE	173	157.260	41.140	58.122	1.00	46.77	. ':	H
ATOM	2966	$\mathbf{cz}$	PHE	173	157.120	42.523	58.097	1.00	50.06	1	Н
ATOM '	2967	С	PHE	173	152.651	39.103	54.870	1.00	51.94	;	H
MOTA	2968	0	PHE	173	152.670	37.881	54.715	1.00	45.37	:	н
ATOM	2969	N .	PRO	174	151.873	39.901	54.128	1.00	47.56	;	H
ATOM	2970	CD	PRO	174	151.760	41.360	54.268	1:00	40.08		H
ATOM	2971	CA	PRO	174··	151.010	39.369	53.070	1.00	39.95	• • ;	H
ATOM	2972	CB	PRO	174	150.417	40.618	52.419	1.00	38.02	• . :	H
· ATOM	2973	CG	PRO	174	151.234	41.778	52.945	1.00	41.70	;	H
MOTA	2974	Ċ	PRO	174	151.793	38.515	52.080	1.00	34.30	•	H
ATOM	2975	Ο.	PRO	174	152.926	38.844	51.719	1.00	38.61	. :	H
MOTA	2976	N	ALA	175	151.191	37.407	51.655	1.00	33.98	;	H
ATOM	2977	CA	ALA	175 .	151.834	36.505 1	50.711	1.00	28.24		Н
ATOM	2978	CB	ALA	175	150.947	35.303	50.455	1.00	24.04		H
MOTA	2979	С	ALA	175	152.106	37.226	49.411	1.00	43.10	;	H·
ATOM	2980	0	ALA	175	151.420	38.182	49.064	1.00	41.83		H
ATOM	2981	N	VAL	176	153.119	36.758	48.691	1.00	47.34		Н
MOTA	2982	CA	VAL	176	153.479	37.340	47.409	1.00	46.04		H
MOTA	2983	CB	VAL .	176	154.660	38.335	47.546	1.00	48.76		H
MOTA	2984		VAL	176	155.822	37.686	48.280	1.00	50.38		H٠
ATOM	2985	CG2		176	155.100	38.809	46.167	1.00	64.07	•	Н
ATOM ·	2986	С	VAL	17Ġ	153.858	36.205	46.462	1.00	36.12		H
MOTA	2987	0	VAL	176	154.544	35.263	46.857	1.00	30.73		H
ATOM	2988	N	LEU	177	153.392	36.298	45.220	1.00	48.02		H
MOTA	2989	CA	LEU	177	153.647	35.282	44.205	1.00	60.32		Н
ATOM	2990	CB	LEU	177 ·	152.686	35.467	43.036	.1.00	39.51		H
ATOM ·	2991	CG	LEU	. 177	152.048	34.165	42.557	1.00	27.99		H
MOTA	2992	· CD1	LEU	177	151.014	33.698	43.572	1.00	30.57		H ·
ATOM	2993	CD2	LEU	177	151.410	34.378	41.197	1.00	38.71		H
ATOM	2994	C ·	LEU	177	155.074	35.257	43.679	1.00	73.61		н.
ATOM	2995	0	LEU	177	155.621	36.275	43.254	1.00	78.42	•	Н
MOTA	2996	N	GLN	178 .	155.669	34.074	43.694	1.00	79.08		H
MOTA	2997	CA	GLN	178	157.031	33.895	43.227	.1.00	95.82		H
ATOM	2998	CB	GLN	178	157.981	33.932	44.432		99:99		H
MOTA	2999	CG	GLN	178	159.244	33.098	44.308		99.99		H
ATOM	3000	CD	Gľ'n	178	160.357	33.583	45.224		99.99		H
ATOM	3001	OE1		178	160.327	33.367	46.439		98.52		H
MOTA	3002	NE2		178	161-350	34.244	44.637		99.99		H
MOTA	3003	C	GLN	178	157.123	32.564	42.483		99.99		H
MOTA	3004	0	GLN	178	157.289	31.504	. 43.092		99.97		H
MOTA	3005	N	SER	179	156.984	32.637	41.159		96.75		H
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MOTA	3007	CB	SER	179	158.307	30.641			93.06		H
MOTA	3008	OG .		179	159.098	30.472	39.425		67.71		H
ATOM	3009	C	SER	179	155.815	30.580	40.430		81.94		H
MOTA	3010	0	SER	179	155.927	29.351	40.461		85.05	•	H
	3011	N	ASP	180	154.649	31.217	40.517		61.79		H H
MOTA	3012	CA	ASP	180	153.367	30.518	40.643		53.42 63.39		Н
ATOM.	3013	CB	ASP	180	153.284	29.372	39.633				H
ATOM	3014	CG	ASP ·	180	152.902	29.846	38.251		90.41		*1

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                                                                                    Н
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                    PRO
         3134
 ATOM
                                                        73.804
                                                                 1.00 46.54
                                                                                    H
                                     167.526
                                               31.972
                            196
                CA
                    PRO
         3135
 ATOM
                                                                                    H
                                               31.339 4 73.154
                                                                 1.00 39.17
                                     168.764
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         3136
                CB
                     PRO
 MOTA
                                                                                    н
                                                                 1.00 48.88
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 ATOM
         3137
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                                                                                    H
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 ATOM
                                                                                    H
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 ATOM
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                O
                                                                                    H
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 MOTA
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                                                                                    Н
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                                                                  1.00 75.74
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 MOTA
                                                                                    H
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                0
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 MOTA
                                                                                    H
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                                                         76.809
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                            198
                N
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 MOTA
                                                                  1.00 57.31
                                                                                    H
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 ATOM
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 MOTA
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                 CG
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                                                32.093
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                                                                                    н
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                                                         77.680
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                     GLU
  MOTA
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                 OE1
                                                                                    Н
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                                                32.725
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                                     160.689
                 OE2
                     GLU
          3152
  MOTA
                                                                                    H
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                 C
                     GLU
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 MOTA.
                                                                                    Ħ
                                                         74.201
                                                                  1.00 63.21
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                            198
                 0
                     GLU
  MOTA
          3154
                                                                                    Н
                                                                  1.00 54.93
                                                         74.614
                                                28.314
                                     162.462
                     THR
                            199
                 N
  MOTA
          3155
                                                                                    H
                                                         73:203
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                                                27.937
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                 CA ·
                     THR
          3156
  ATOM
                                                                                    н
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                                      162.304
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                 CB
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                                                                                     H
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                                                                  1.00 78.07
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  MOTA
                                                                  1.00 59.63
                                                                                     H
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                                                28.583
                            199
                      THR
          3160
                 C
  MOTA
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                                                                                     H
                                                         73.054
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                      THR
                            199
          3161
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                                                                                     H
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                                      160.407
                      VAL
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          3163
                 CA
                                                                                     Н
                                                         70.035
                                                                   1.00 33.42
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          3164
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          3165
                 CG1
                     VAL
  ATOM
                                                                                     Н
                                                31.944
                                                         71.239
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                             200
                      VAL
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          3166
                 CG2
                                                                                    ,H
                                                         69.112
                                                                   1.00 51.65
                                                28.832
                                      160.195
                             200
                      VAL
          3167
                 C
  ATOM
                                                                                     H
                                                         68.353
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                                                28.613
                                      161.136
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          3168
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                                                                                     н
                                                          68.862
                                                                   1.00,39.44
                                                28.427
                      THR
                             201
                                      158.955
                 N
          3169
  ATOM
                                                                                     H
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                                                                   1.00 32.31
                                                27.684
                             201
                                      158.631
                      THR
                ·CA
          3170
  MOTA
                                                                                     H.
                                                26.267
                                                          67.969
                                                                   1.00 41.49
                             201
                                      158.116
                      THR
          3171
                 CB
  MOTA
                                                                                     Н
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                                                          68.831
                                                 25.602
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                      THR
                             201
                 OG1
  MOTA
          3172
                                                                                     H
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                                                                  1.00 39.87
                                                 25.458
                                      157.949
                      THR
                             201
                 CG<sub>2</sub>
           3173
  MOTA
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٠.	•						28.399	66.860	1.00 2	26.58		H
MOTA	3174	C .	THR	201		157.545	29.055	67.438	1.00			· H
MOTA	3175	0	THR	201		156.682	28.279	65.538	1.00			H
MOTA	3176	N	CAR	202			28.279	64.699	1.00			H
MOTA	3177	CA	CYS .	-		156.582	27.777	64.064	1.00			н .
MOTA	3178	C	CYS	202		155.765	26.826	63.522	1.00			H
MOTA	3179	0	CYS	.505		156.324		63.522	1.00			H .
MOTA	3180	CB	CYS	202.			29.820	61.983	1.00			H.
ATOM	3181	SG	CYS	202		157.564	29.150		1.00			н
MOTA	3182	и.	ASN	203		154.441	27.871	64.172 63.628	1.00			н
MOTA	3183	CA	asn	203		153.554	26.842	64.686	1.00			H
ATOM	3184	CB	nra	203		152.539	26.387	, ,	1.00			н
ATOM	3185	·CG	ASN	. 203		152.926	26.807	66.099	1.00			H
ATOM	3186	ODl	ASN	203	•	152.586	27.904	66.552	1.00			H
ATOM	3187	ND2	ASN	203		153.629	25.926	66.805	1.00			н
MOTA	3188	C	ASN	203		152.800	27.293	62.389		38.03		н
MOTA	3189	0	ASN	203		151.964	28.196				•	н
MOTA	3190	N	VAL	204			26.646	61.270		23.45 38.87	•	н
ATOM .		CA	VAL	204		152.451		60.006				H
ATOM		CB	VAL	204	•	153.473	27.049	58.853		39.50		н
ATOM	3193		VAL	204		152.795	27.575	57.599		52.52		н
MOTA	3194	CG2		204		154.624		59.254		29.99		H
ATOM	3195	С	VAL	204		151.461	25.854	59.676		41.89		н
ATOM	3196		VAL	204		151.733	24.682	59.919		46.77		H
ATOM	3197	Ŋ	ALA	205		150.312	26.236	59.126		41.52		
ATOM	3198	CA	ALA	205		149.285	25.273	58.751		32.14		H
ATOM	3199	CB	ALA	205		148.156	·25.281			44.74		·H
ATOM	3200	C		205		148.749	25.614	57.365		28.16		H
ATOM	3201	Ō	ALA	205		148.349	26.750	57.104		23.06		H
ATOM	3202	N	HIS	. 206		148.756	24.629	56.474		38.89		H
MOTA	3203	CA	HIS	206	٠	148.267	24.825	55.121		31.01		. н
ATOM	3204	CB	HIS	206		149.357	24.497	54.112		34.08		. н
ATOM	3205	CG	HIS	206	•	149.025	24.909	52.715		25.51		H
MOTA	3206		HIS	206		148.521	26.065	52.227		33.37		· H
MOTA	3207		HIS	206	•	149.193	24.073	51.635		28.36		H
ATOM	3208		HIS	206		148.807	24.698	50.535		30.36		H
MOTA	3209		HIS	206		148.393	25.907	50.868		29.53		H
ATOM	3210		HIS	206		147.061	23.930	54.876		38.48		H.
ATOM	.3211		HIS	206		147.198	. 22.819			42.18		H
ATOM	3212		PRO	207		145.856	24.417			46.11	•	H.
ATOM	3213		PRO	207		145.636	25.758			59.24		H
MOTA	3214			207		144.597	23.684			49.09		
MOTA	3215		PRO	207		143.538	24.780			55.68		. н
	3216		PRO	207		144.146	25.814			65.42		H
MOTA MOTA	3217		PRO	. 207		144.504	22.890	53.769		60.16		Н
	3218		PRO	207		144.293				51.48		H
ATOM	3219		ALA	208		144.664	23.577			56.11		. н
MOTA	3220					.144.584	22.933			41.51		, H
MOTA	3221					145.043	23.899			34.52		- H
MOTA	3222	-	ALA			145.397				43.41		• Н
ATOM	3223		ALA			144.983				51.37		H
MOTA	3224		SER			146.550		51.93		47.62		`. H
ATOM	_		•			147.396				48.72		H
ATOM	322				٠.	148.852		L 51.634	1.00	44.67	•	H
MOTA	3220			•					•	•		••

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MOTA	3227	QG.	SER	209	149.387	21.642	52.650	1.00 55.80	, , <b>н</b> Н
ATOM	3228	C	SER	209	147.304	19.643	53.236	1.00 53.29 1.00 52.35	H <sub>.</sub>
MOTA	3229	0	SER	209	147.973	18.624	53.411	1.00 52.35	H
MOTA	3230	N	SER	<b>Ż10</b>	146.462		54.148	1.00 71.17	н.
MOTA	3231	CA .	SER	210	146.269	19.475	55.444	1.00 90.95	н
MOTA	3.232	CB	SER	210	145.509	18.158	55.277	1.00100.00	H
MOTA	3233	OG	SER	210	144.137	18.333	55.578	1.00100.00	н
ATOM	3234	С	SER	.210	147.579	19.213	56.169	1.00 79.39	. н.
ATOM	3235	0	SER	210	147.702	18.234	56.908	1.00 73.59	н
ATOM .	3236	Ŋ	THR	211	148.555	20.088	55.950	1.00 75.14	H.
MOTA	. 3237	CA	THR	211	149.854	19.964	56.594	1.00 76.28	H
MOTA	3238	CB	THR	211	151.027	20.111	55.599	1.00 73.28	· H
MOTA	3239	OG1		211	150.990		55.008	1.00 73.03	H
MOTA	3240	CG2	THR	211	150.950	19.062	54.510	1.00 74.45	H.
ATOM	3241	C.	THR	211	150.024	21.051	57.643	1.00 74.45	н -
ATOM	3242	0	THR	211	149.536	22.17.2		1.00 70.05	н,
ATOM	3243	N	LYS	212	.150.711		58.722	1.00 61.67	Н
MOTA	3244	CA	LYS	212	150.988	21.645	59.783	1.00 73.38	н
MOTA '	3245	CB	LYS .	212	150.041	21.450	60.967	1.00 75.50	н
MOTA	3246	CĠ	LYS	212	150.718	21.612			н
MOTA	3247	CD	LYS	212	150.006		63.192	1.00 97.52	H.
MOTA	3248	CE	LYS	212	150.452	22.449	64.637	1.00 97.32	, H
MOTA	3249	NZ	LYS .	212		.23.707	65.419	1.00 51.18	н
MOTA	3250	C	LYS	212	152.413		60.198 60.594	1.00 31.10	H
MOTA	3251	Ο.	LYS	212	. 152.730	20.222	60.594	1.00 47.52	н
MOTA	3252	N	VAL	213	153.275	22.349	60.434	1.00 47.32	н
MOTA	⋅ 3253	CA	VAL	213 .	154.672	22.201	59.282	1.00 35.68	,H
MOTA	3254		VAL	213	155.593	22.651	59.511	1.00 51.97	H
ATOM.	3255		VAL	213	157.002	22.136	57.948	1.00 53.21	• н
MOTA	3256		VAL	213	155.047	22.154	61.661	1.00 30.06	H
MOTA	3257	G.	VAL	213	155.011	23.028	61.991	1.00 34.34	H
ATOM.	3258	0	VAL	213	154.324	23.996	62.343	1.00 35.26	н
MOTA	3259	Ŋ	ASP	214	156.071	23.325	63.523	1.00 39.19	н
MOTA	3260	CA	ASP	214	156.541	22.526	64.791	1.00 58.41	Ĥ
ATOM .	3261	CB	ASP	214	156.228	22.709	65.259	1.00 63.54	. н
MOTA	3262	CG	ASP	214	154.791	23.857	65.553	1.00 65.10	н
MOTA	3263		ASP	214	154.397 154.059	23.637	65.336		. н
MOTA	3264		ASP	214	158.046	23.454	63.342	1.00 37.64	. н
MOTA	3265	G.	ASP	214	158.725		62.983	1.00.41.00	. н
MOTA	3266	.0	ASP	214	158.725	24.652	63.564	1.00 34.85	н
MOTA	3267	. N	LYS	215	159.985	24.877	63.410	1.00 35.83	н
MOTA	3268	CA	LYS	215 215	160.261	25.637	62.112	1.00 37.75	H
MOTA	3269	CB	LYS		161.248	24.948	61.191	1.00.59.89	H
MOTA	3270	CG	LYS	215 215	160.536	23.992	60.251		H.
ATOM	3271	•	LYS		161.386	22.766		1.00 53.98	: н
MOŢA	3272	CE	LYS	215 215	160.573	21.613	59.475	1.00 65.45	н
MOTA	3273	NZ	LYS	215	160.575	25.659	64.588		н
MOTA	3274	C	LYS	215	160.030		64.904		н
MOTA	3275		LYS	215	161.511		65.244		H
MOTA	3276		LYS	. 216	162.141		66.389		. <b>H</b>
MOTA			LYS	216	162.649		67.357		H
MOTA	3278			216	162.043	·	67.119		. <b>H</b>
ATOM	3279	CG	<b>LYS</b>	5 i 0	102.043			• .	

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1.00 85.40
                                            22.156
                                                     67.793
                                  162.861
                   LYS
       3280
              CD
MOTA
                                                              1.00 94.97
                                           .22.085
                                                     69.296
                                  162.592
                         216
                  LYS
        3281
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MOTA
                                                              1.00 92.19
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MOTA
        3282
              ΝZ
                                                              1.00 46.24
                                                                                H
                                                     65.860
                                             26.543
                                  163.305
                        : 216
                   LYS
        3283
              C
MOTA
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                                                              1.00 34.41
                                                     64.838
                                 . 163.898
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                         216
                   LYS
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MOTA
                                                                                Н
                                                              1.00.41.02
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                                                     66.541
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MOTA
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                                                              1.00 44.97
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                   ILE
MOTA
        3286
                                                                                H
                                                              1.00 41.86
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                                                     66.046
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MOTA
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                                                                                 н.
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ATOM
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                                                                                 H
                                                              1.00 33.66
                                   162.768
                                                     65.749
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              CG1. ILE
                          217
MOTA
        3289
                                                                                 Ħ
                                                               1.00 17.95
                                   162.407
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                                                     . 64.270
                          217
              CD1 ILE
        3290
MOTA
                                                                                 H
                                                               1.00 47.47
                                                      67.094
                                  165.890
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                   ILE
        3291
               C
MOTA
                                                                                 Н
                                                               1:00 43.27
                                                     68.310
                                             28.400
                                   165.690
                          217
                   ILE
        3292
               O
MOTA
                                                                                 H
                                                               1.00 50.40
                                                      66.559
                                             28.219
                                   167.103
              N
                   VAL
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MOTA
                                                                                 H
                                                               1.00 50.95
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               CG1 VAL
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MOTA
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                          218
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               CG2 VAL
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MOTA
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MOTA
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ATOM
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MOTA
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                                                      47.685
                                             32.588
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ATOM
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                                                      46.699 1.00 53.80
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                                    95.825
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               CG
. ATOM
                                                               1.00 62.43
                                                                                 C
                                             30.925
                                                      46.486
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                            2
         3303
 MOTA
                                                               1.00 62.95
                                                                                 C
                                                      45.531
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                                    94.373
               CE
                             2
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                   LYS
 ATOM
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                                                               1.00 60.28
                                                      46.232
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                                     94.065
                             2
         3305 NZ
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MOTA
                                                                                  C
                                                      .49.840 . 1.00 46.91
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 MOTA
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                                                               1.00 58.66
                                                      50.239
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                                     93.606
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                             2
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 MOTA
                                                                                  C
                                                               1.00 34.71
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                                                       49.234
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               N
                    LYS
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 MOTA
                                                                                  C
                                                               1.00 47.34
                                                       49.150
                                     95.690
                                              32.169
                             2
               CA
                    LYS
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 ATOM
                                                                                  C
                                                      49.975
                                                               1.00 39.77
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                                     95.072
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               N
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         3310
 MOTA
                                                                                  C
                                                                1.00 41.61
                                                      50.621
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						54.941	50.502	1.00 25.92	C.
MOTA	3439	0	ASN	19	91.113	54.446	50.781	1.00 37.11	C
MOTA	3440	N	LEU	20 .	93.291	53.097	50.204	1.00 39.33	С
MOTA	3441	CA	LEU	20	93.192	52.830	49.284	1.00 52.73	C
MOTA	3442 .	CB	LEU	20	94.382	53.492 ·	47.913	1.00 59.34	C,
ATOM :	3443	CG	LEU ·	20	94.409 95.375	54.657	47.953	1.00 54.35	C
MOTA	3444			. 20	95.3/5	52.478	46.855	1.00 58.17	C
MOTA	3445	CD2	LEU	20	93.122	51.946	51.202	1.00 24.88	C
ATOM	3446	C.	LEU	20	93.122	51.349	51.532	1.00 27.29	C
MOTA	3447	0	LEO .	20	91.926	51.619	51.670	1.00 24.25	C
MOTA	3448	N	ŞER	. 21	91.795	_	52.601	1.00 32.93	C
MOTA	3449	CA	SER	21	90.474	50.603	53.357	1.00 22.84	C
MOTA	3450	CB	SER	21	90.626		54.682	1.00 42.82	C
MOTA	3451	OG.	SER	21	91.834	49.250	51.760	1.00 36.87	C
MOTA	3452	C	SER.	21	91 633	49.308	50.551	1.00 50.83	, <b>C</b>
MOTA	3453		SER	21 22	92.098	48.109	52.384	1.00 41.84	, C
MOTA	3454	N	CYS	22	92.142	46.858	51.636	1.00 34.97	C
MOTA	3455	CA	CYS	22	91.519	45.728	52.420	1.00 29.54	· с
MOTA	3456	C	CYS	22	92.086		53.400	1.00 31.51	C
MOTA	3457	0.	CYS	22	93.578	46.504	51.294	1.00 44.42	C
MOTA	3458	CB	CYS CYS	22 .	94.382	47.674	50.162	1.00 54.15	
MOTA	3459	SG	LYS	23	90.339	45.312	51.983		. G
ATOM	3460	N CA	LYS	23	89.630		52.639	1.00 27.48	C
ATOM	3461			23	88.196	_	52.099	1.00 45.60	C
ATOM	3462	CB CG	LYS	. 23	87.083		53.160	1.00 46.91	C
ATOM	3463	CD.		23	. 85.742		52.558	1.00 49.03	. C
ATOM	3464	CE		23	84.537	43.911	53.219	1.00 44.60	· C
MOTA	3465 3466		LYS	23	83.321			1.00 31.56	· · · · · · · · · · · · · · · · · · ·
MOTA	3467	C	LYS	23	90.373	42.933	52.354	1.00 28.04	C
MOTA	3468		LYS	23	90.727	42.651	51.209	1.00 27.74	C
MOTA	3469	И	TYR	24	90.616	42.154		1.00 48.19	C
MOTA	3470	CA		24	91.305		53.279		C
ATOM .	3471	CB		24	.92.585	40.864	54.121		· C
MOTA	3472	CG		24	93.582	41.914	53.708		c
MOTA MOTA	3473		1 TYR	24	94.190	41.867	52.454		
ATOM	3474		1 TYR	24	95.089				c
ATOM	3475			24	93.90				Ċ
ATOM	3476			24	94.80				Ċ
ATOM	3477			24	95.38				, c
ATOM	3478			24 ·	96.26				Ċ
ATOM	3479		TYR	24		3. 39.736	53.749		. c
ATOM	3480		TYR	24	89.26				c
ATOM	3481		SER	. 25	90.92				. с
MOTA	3482			25	90.17				: с
ATOM	3483	CI	SER	25	89.88				' с
MOTA	3484	. 00	3 SER	. 25	91.06				C
ATOM	3485	C	SER	25	91.07				. C
ATOM	3486		SER	25	91.29				c
MOTA	3487	7 N		26	91.60				- c`
ATOM	3488	3 C		26	92.51				
ATOM	3489	9 C		26	.93.94	_			, c
ATOM					94.84				. с
MOTA		1 C	D1 TYR	26	95.60	. 30.02		•	•
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1.00 50.14
                                            35.003
                                                     58.673
                                   96.443
                          26
MOTA
       3492
                                                              1.00 43.23
                                                     56.363
                                            34.677
                                   94.941
                          26
       3493
              CD2
                  TYR
                                                                                 C
MOTA
                                                              1.00 62.28
                                                     56.809
                                            33.646
                                   95.776
                          26
              CE2
                  TYR
       3494
                                                                                C
MOTA
                                                              1.00 56.86
                                            33.816
                                                     57.964
                                   96.524
                          26
                  TYR
       3495
              CZ
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MOTA
                                                              1.00 54.48
                                           32.801
                                                     58.404
                                   97.352
                          26
                  TYR
       3496
              OH
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MOTA
                                                              1.00.30.34
                                            37.637
                                                     58.451
                                    92.455
                          26
                  TYR
       3497
              C
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MOTA
                                                              1.00 12.16
                                                     58.518
                                            38.851
                                    92.275
                          26
       3498
              O
                  TYR
                                                                                 C
MOTA
                                                              1.00 35.16
                                             36.832
                                                     59.504
                                    92.626
                          27
        3499
              N
                   ASN
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MOTA
                                                              1.00 · 43.53
                                                     60.920
                                            37.230
                                    92.639
                           27
                   ASN
        3500
              .CA
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MOTA
                                                               1.00 44.74
                                    94.092
                                                      61.380
                                             37,461
                           27
                   ASN
              CB
ATOM
        3501
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                                                               1.00 54.71
                                                      61.095
                                    94.595
                                             38.869
                   ASN
                           27
              CG
        3502
                                                                                 C
ATOM
                                                              1.00 49.86
                                            39.691
                                                      60.503
                                    93.890
                           27
              OD1. ASN
       3503
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ATOM.
                                                               1.00 38.35
                                                      61.521
                                    95.833
                                             39.153
                           27
              ND2 ASN
        3504
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ATOM
                                                               1.00 52.07
                                                      61.413
                                    91.760
                                             38.379
                           27
                   ASN
        3505
              С
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ATOM
                                                               1.00 64.58
                                                     .60.582
                                             39:159
                                    91.255
                   ASN
                           27
        3506
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MOTA
                                                               1.00 38.64
                                                      62.651
                                             38.478
                                    91.583
                   ASN
                           27
              OT
        3507
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MOTA
                                                               1.00 38.67
                                                      66.273
                                    98.029
                                             39.101
                           30
               CB
                   SER
        3508
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MOTA
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                                                      66.371
                                             39.940·
                                    99.164
                           30
                   SER
        3509:
              OG
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MOTA
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                                                      64.527
                                             37.741
                                    99.198
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                   SER
MOTA
        3510
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                                                      65.163
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                                    99.534
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                   SER
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MOTA
        3511
                                                               1.00 40.61
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                                                      64.847
                                            37.537
                                    96.758
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               N
                   SER
        3512
                                                                                  C
                                                               1.00 46.89
MOTA
                                                      64.881
                                             38.480
                                    97.910
                           30
        3513
               CA
                    SER
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                                                               1.00 52.76
MOTA
                                                      63.505
                                             38,226
                                    99.906
                           31
                    ARG
               N
        3514
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                                                               1.00 48.62
MOTA
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                                             37.606
                                 101.156
                           31
                    ARG
               CA
        3515
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MOTA
                                                               1.00 48.21
                                                       62.014
                                             36.509
                                    100.864
                    ARG
                           31
               CB
        3516
                                                                                  C
 ATOM
                                                                1.00 45.83
                                              36.316 61.654
                                     99.390
                            31
        3517
               CG
                    ARG
                                                                                  C
 MOTA
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                                              34.913
                                                       61,098
                                     99.123
                            31
        3518
               CD
                    ARG
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 MOTA
                                                                1.00.56.80
                                                       61.946
                                              34.159
                            31
                                   98.202
                    ARG
               ΝE
        3519
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 MOTA
                                                                1.00 60.88
                                              32.904 61.723
                                     97.819
                            31
                    ARG
               CZ
        3520
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 MOTA
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                                                       60.666
                                     98.273 . 32.238
                            31
               NH1 ARG
        .3521
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 MOTA
                                                       62.565
                                                                1.00 65.41
                                              32.312
                                     96.980
                            31
                NH2
                   ARG
         3522
 MOTA
                                                                1.00 42.34
                                                       62.457
                                    102.140. 38.620
                    ARG
                            31
                C
         3523
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 MOTA
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                                                                1.00 37.05
                                    102.024 39.821
                            31
                    ARG
         3524
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                                                                1.00 33.63
 MOTA
                                                       61.688
                                    103.109
                                              38.119
                    GLU
                            32
                N
         3525
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 MOTA
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                                              38.959
                                                       61.035
                                    104.114
                            32
                CA
                    GLU
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         3526
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 MOTA
                                                       61.211
                                              38.366
                                    105.510
                            32
                CB
                    GLU
         3527
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 MOTA
                                                                1.00 44.46
                                                       60.762
                                              39.289
                                    106.639
                            32
                    GLU
                CG
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 MOTA
         3528
                                                                1.00.47.94
                                              38.584
                                                       60.704
                                    107.993
                    GLÜ
                            32
                ĊD
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         3529
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 MOTA
                                                       61.436
                                              37.588
                                    108.183
                            32
                OE1
                    GLU
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         3530
 ATOM
                                                                1.00 43.16
                                    108.870 39.024
                                                       59.931
                            .32
                OE2 GLU
         3531
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 ATOM.
                                                                1.00 32.96
                                                       59.550
                                              39.047
                                    103.777
                            32
                    GLU
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                C
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 MOTA
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                                              38.061
                                    103.876
                             32.
                     GLU
         3533
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 MOTA
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                                                       59.122
                                     103.394 40.244
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 ATOM
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                                                                 1.00 35.05
                                    102.989
                                               40.488
                     PHE
                             33
         3535
                CA
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  MOTA
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                                     101.494
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 MOTA
         3536
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                                                                 1.00 24.17
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                             33
                     PHE
  MOTA
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                CG
                                                                 1.00 23.40
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                                               43.192
                                     101.369
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                CD1 PHE
         3538
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  ATOM
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                CD2
  ATOM
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                                     100.989
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                CEL
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          3540
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  MOTA
                                                                 1.00 31.35
                                                        59.703
                                               44.304
                                     100.292
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                 CZ
                    PHE
         3542
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  MOTA
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                                                                 1.00 34.54
                                               41.716
                                     103.640
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                     PHE
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  MOTA
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                                               42.613
                                     104.134
                     PHE
          3544
  MOTA
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	. •								С
NTOM	3545	N A	RG	34			55.797 1 55.045 1	00 28.28	c
ATOM	3546	CA A	RG	34				00 12.61	Ċ
MOTA	3547	CB P	LRG '	34				00 19.39	Ċ
ATOM ·	3548	CG F	ARG	. 34	106.189	43.483		.00 18.93	Ċ
ATOM .	3549	CD F	ARG ·	34		42.916	-	1.00 36.83	С
MOTA	3550	NE A	ARG	34 .	108.026	43.440		1.00 40.83	. C
ATOM	3551	CZ I	<b>ARG</b>	34	. 108.251	44.344		L.00 45.97	Ċ
ATOM	3552		ARG	34	107.239	44.825		1.00 38.52	Ċ
ATOM	3553		ARG	34		44.752		1.00 32.95	Ċ
ATOM	3554	c z	ARG	34	103.202	43.309		1.00 41.93	C.
MOTA	3555		ARG	34	103.239	42.779	-	1.00 34.63	c
ATOM	3556	N i	ALA '	-35	102.362	44.294	=	1.00 26.09	С
ATOM	3557	CA	ALA	35	101.416	44.798		1.00 26.37	C
ATOM .	3558	CB·	ALA	35	100.381	45.657		1.00 28.19	Ċ.
MOTA	3559	C.	ALA	35	102.134	45.599		1.00 20.23	C
ATOM	3560		ALA	35	103.201	46.163		1.00 15.20	· c
ATOM	3561		SER	36	101.545	45.641		1.00 30.37	Ċ.
ATOM	3562		SER	36	102.136	46.374	• •	1:00 51.82	· C
ATOM	3563		SER ·	36 .	103.172	45.488		1.00 51.82	Ċ
ATOM .	3564		SER	36	103.705	44.516	50.050	1.00 82.37	Ċ
ATOM	3565	C	SER.	36	101.099	46.886	48.847	1.00 32.13	Ċ
ATOM	3566	ō	SER	36	100.092	46.238	48.575	1.00 28.44	. c
ATOM	3567	N.	LEU	37	101.364		48.304	1.00 31.61	· c
ATOM .	3568	CA:	LEU	37	100.496	48.705	47.320	1.00 31.61	Ċ
ATOM	3569	CB	LEU	37	99.897	49.987	47.895	1.00 36.64	c
ATOM	3570	CG	LEU	37	98.943	50.801	47.023	1.00 21.57	Č
ATOM	3571		LEU	37	97.533		47.578	1.00 26.43	Ċ
MOTA	3572	· CD2	LEU	37	99.412	52.231	46.991	1.00 28.45	, c
ATOM	3573		LEU	37	101.393	49.042	46.148	1.00 25.00	Ċ
ATOM	. 3574	•	LEU	37	102.341	49.811	46.295	1.00 33.13	, c
ATOM	3575			38	101.112	48.454	44.993	1.00 21.00	Ċ.
ATOM	3576		HIS	38	101.935	48.694	43.816	1.00 29.80	Č
ATOM	3577		HIS	38	102.418	47.370	43.232	1.00 41.65	C
ATOM	3578		HIS	38	103.038	46.464	44.248	1.00 36.66	. 'C
ATOM	3579		HIS	38	104.324	46.102		1.00 51.35	· с
ATOM	3580		HIS	38	102.296	45.819		1.00 45.79	· c
ATOM			HIS	. 38	103.102	45.102		1.00 50.11	C
ATOM	3582		HIS	38	104.337			1.00 20.21	С
ATOM	3583		HIS	.38	101.138	49.458		1.00.24.62	Ċ
ATOM	3584		HIS	38	99.935			1.00 17.62	С
MOTA	. 3585		LYS	39	101.807			1.00 28.42	, .C
ATOM	3586		LYS	39.	101.135			1.00 33.83	· C
ATOM	. 3581		LYS	39	101.458			1.00.47.76	, C
ATOM	358		LYS	39	100.938			1.00 56.33	C
MOTA	358	e CD	LYS	39	102.046			1.00 52.05	. c
ATOM		O CE	LYS	39	101.922			1.00 39.26	С
ATOM		1 NZ	LYS	39	101.573			1.00 37.38	. с
ATOM			LYS	39			`	1.00 38.26	С
ATOM		_	LYS	39	102.715			1.00 33.72	С
ATOM	•	4 N	$G\Gamma\Lambda$	40	100.528				C
ATOM		S CA		40	100.819				C
ATOM			GLY	40	100.18			•	C
ATOM		7 0	GLY	40	100.02	5 47.99	, 3,		

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MOTA	3598 ·	N	LEU	41	99.819	48.962	35.634	1.00 48.13	Ċ
MOTA	3599	CA	LEU	41	99.196	47.809	34.988	1.00 43.35	C
MOTA	3600	СВ	LEÜ	. 41	98.598	48.211	33,633	1.00 41.37	C .
MOTA	3601	CG	LEU	41	97.256	47.613	33.178	1.00 50.66	
MOTA	3602	CD1	LEU	41	96.622	46.783	34.283	1.00 41.32	C
MOTA	3603	CD2	LEU	41 .	96.324	48.742	32.756	1.00 36.16	, G
ATOM	3604	C	LEU	41	100.270	46.758	34.791	1.00 44.95	
MOTA	3605	0	LEU	41	99.976	45.585	34.577	1.00 48.29	C
MOTA	3.606	N	ASP	42 .	101.522	47.197	34.841	1.00 51.52	C
MOTA	3607	CA	ASP	42	·102.648	46.285	34.713	1.00 53.82	C
MOTA	3608	CB	ASP	42	103.666	46.804	33.690	1.00 44.60	C
ATOM	3609	CG	ASP	42	104.352	48.090	34.125	1.00 49.55	C
MOTA	3610	ODl	ASP	42	103.874	48.765	35.063	1.00 40.26	C
ATOM	3611	OD2	ASP	42	105.385		33.510	1.00 48.33	C
ATOM	3612	C	ASP	42	103.249	46.241	36.106	1.00 57.65	C
MOTA	3613	0	ASP	. 42	104.394	45.836	36.298	1.00 57.61	. C
ATOM	3614	N	SER	43	102.433	46.679	37.065	1.00 57.54	C
MOTA	3615	CA	SER	43	102.767	46.741	38.486	1.00 56.75	. C
MOTA.	3616	CB	SER	43.	102.299	45.467	39.177	1.00 40.78	. C
MOTA	3617	OG	SER	<b>43</b> .	100.896	45.502	39.359	1.00 32.86	. с
MOTA	3618	С	SER	43	104.234	46.995	38.803	1.00 59.27	C
ATOM	3619	0	SER	43 .	104.795	46.413	39.732	1.00 57.66	C
ATOM	3620	N	ALA	44	104.847	47.884	38.033	1.00 54.64	c
ATOM	3621	CA	ALA	44	106.244	48.215	38.224	1.00 41.67	
MOTA	3622	CB	ALA	44	106.654	49.295	37239	1.00 41.38	. с
MOTA	3623	C	ALA	44	106.514	48.679	39.646	1.00 42.01	·C
ATOM	3624	0	ALA	44	107.073	47.935	40.449	1.00 48.39	
MOTA	3625	N	VAL	45	106.083	49.904	39.943	1.00 40.52	C.
MOTA	3626	CA		45	106.290	50.563	41.239	1.00 34.97	
ATOM		CB	VAL	45	106.036	52.073	41.094	1.00 27.80	
MOTA	3628		VAL	45	106.126	52.753	42.441	1.00 32.20	Ċ
ATOM '	3629	.CG2	VAĻ	45	107.036	52.674	40.126	1.00 35.71	c
ATOM	3630	C	· VAL	45	105.526	50.100	42.489	1.00 35.47	c
MOTA	3631	0	VAL	45	104.307	49.956	42.462	1.00 39.87	
MOTA	3632	N	GLU	46	106.259	49.893	43.585		c
ATOM	3633	CA	GLU	46	105.666	49.503	44.868	1.00 50.85	c
ATOM	3634	CB	GLU .		106.546	48.488	45.615	1.00 34.64	. c
ATOM	3635	CG	GLU	46	106.163	48.251	47.094	1.00 57.55	c
MOTA	3636	CD	GLU	46	106.638	46.895	47.637		C
MOTA	3637		. GLU	46	107.869	46.712	47.809 47.893		
MOTA	<b>઼3638</b>		GLU	46	105.783	46.014	45.680	1.00 23.27	C
MOTA	3639	C	GLU		105.575	50.791	46.338	1.00 43.67	Ċ
MOTA	3640	0	GLU	46 .	106.530	51.189	45.614	1.00 25.13	c
MOTA	3641	N.	VAL	47	104.418	51.433 52.692	46.297	1.00 25.13	c
MOTA	3642	CA	VAL	47	104.173		46.037	1.00 19.37	· c
MOTA	3643	CB	VAL	47	102.736	53.146	46.826	1.00 28.90	_
ATOM	3644		L VAL	47	102.428	54.405	44.547		c
MOTA	3645		VAL	47	102.543	53.374 52717		1.00 20.00	c
MOTA	3646	C	· VAL	47	104.437	53:641	48.310	_	Ċ
MOTA	3647	0	VAL	47	105.070	51.709	48.512		c
MOTA	3648	N	CYS	48	103.952 104.142	51.709	49.955		C
MOTA	3649	CA	CYS	48	104.142	50.246			· c
MOTA	3650	С	CYS	48	104.143	JU.240	30.220		

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MOTA	3651	Ο.	CYS .	48	103.618	49.331	49.864	1.00 20.24	c
MOTA	3652	CB	CYS	48	103.035	52.459	50.644	1.00 57.93	· с
MOTA	3653	SG ·	CYS	48	103.314	52.822	52.407	1.00 69.94	. с с
MOTA	3654	N	VAL	49	104.747	50.070	51.664	1.00 18.58	
MOTA	3655	CA	VAL	49	. 104.802	48.764	52.290	1.00 20.44	C
MOTA	3656	CB	VAL	49	106.139	48.030	51.966	1.00 27.56	C
MOTA	3657	CG1	VAL	49	107.042	48.931	51.131	1.00 18.34	C
MOTA	3658	CG2	VAL	49	106.851	47.592	53.249	1.00 17.63	C C
MOTA	3659	C	VAL	49	104.654	48.926	53.794	1.00 33.14	c
MOTA	3660	0	VAL	. 49	105.537	49.471	54.455	1.00 29.92	
ATOM	3661	N	VAL	<b>50</b> .	103.523	48.467	54.324	1.00 41.12	. C
MOTA	3662	CA	VAL	50	103.255	48.539	55.759	1.00 44.37	C
MOTA	3663	CB	VAL	50	101.796	48.932	56.031	1.00 48.04	
MOTA	3664	CG1	VAL	50 ·	101.486	48.786	57.511	1.00 45.70	C
ATOM	3665	CG2	VAL	50	101.562	50.367	55.576	1.00 35.76	c
MOTA	3666	C	VAL	50	103.553	47.176	56.385	1.00 38.20	
MOTA	3667	0	VAL	50	102.899	46.176	56.085	1.00 36.51 1.00 25.60	C
MOTA	3668	N	TYR	51	104.543	47.146		1.00 25.60	c
MOTA	3669	CA	TYR	51	104.957	45.898		1.00 34.11	C
ATOM	3670	CB	TYR	51	106.479	45.779	57.799	1.00 31.19	C
MOTA	3671	CĠ	TYR	51	107.060	44.744	58.724 59.944	1.00 31.13	Ċ
MOTA	3672	CD1		51	107.617	45.109		1.00 44.07	c
MOTA	3673		TYR	51	108.122	44.153	58.395	1.00 33.29	Ċ
MOTA	3674	CD2		51	107.025	43.396	59.265	1.00 33.23	Ċ
MOTA '	3675	CE2		51	107.525	42.432	60.477	1.00 41.02	Ċ
MOTA	3676·		TYR	51 ·	108.068	42.818	61.364	1.00 33.00	. c
ATOM	3677	OH	TYR	. 51	108.511	41.867 45.729	59.315	1.00 33.68	c
MOTA	3678	C	TYR	51,	104.507		60.145	1.00 33.50	Ċ
MOTA	3679	.0	TYR	51	104.696	46.613	59.603	1.00 29.01	C.
ATOM	3680	·N	GLY	52	103.927	44.571	60.947	1.00 30.05	Ċ
ATOM	3681		GLY	52	103.459	43.041	61.527	1.00 39.73	Č.
MOTA	3682	C	GLY	52	104.067	42.096	60.806	1.00 40.35	C
ATOM .	3683		GLY	52 53	104.393	43.032	62,843	1.00 46.66	C
MOTA	3684	N	ASN	53 53	104.224 104.798		63:537	1.00 57.56	C
ATOM	3685	CA	ASN	.53 53	106.308	42.073	63.721	1.00 32.73	C
MOTA	3686	CB	ASN	53	106.971	40.851	64.322	1.00 30.74	С
MOTA	3687	CG	ASN	.53 53	106.474	39.728	64.185	1.00 25.99	G.
ATOM	3688		ASN	53 53	108.099	41.059	64.995	1.00 35.70	С
ATOM	3689		ASN ASN	· 53	104.141	41.729	64.897	1.00 63.15	C
MOTA	3690	₾.	· ASN	53	104.709	42.114	65.918	1.00 67.81	. С
ATOM	3691	•	TYR	54	102.941	41.159	64.906	1.00 66.70	C
ATOM	3692	N CA	TYR	54	102.213	40.953	66.149	1.00 70.87	C
ATOM	3693	CB	TYR	54	103.004	40.008	67.072	1.00 60.20	C Ì
ATOM	369 <u>4</u> 3695	CG	TYR	5 <u>4</u>	103.185	38.604	66.521	1.00 54.18	. С
ATOM			L TYR	54	104.380		65.923	1.00 49.72	C
ATOM	3696		LTYR	54	104.538	36.931	65.393	1.00 51.50	C
MOTA	3697		2 TYR		102.149	37.672	66.579	1.00 63.25	C
ATOM	3698 3699	CE2		. 54	102.297	36.386	66.052		C
ATOM	3699 3700	.CZ	TYR	54 ·	103.489	36.025	*	1.00 51.26	C
MOTA	3700	OH.	TYR	54	103.625	34.761	64.931	1.00 41.36	. c
MOTA	3701 3702	C	TYR		. 102.018	42.313	66.811		C
MOTA	3702	0	TYR	54	101.118	43.072	66.443	1.00 70.77	, c
ATOM	3/03	•	4	<del>-</del> -	•		•	•	

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MOTA	3704	N	SER	55	102.870	42.617	67.784	1.00 89.21	Ċ
MOTA	3705	CA	SER	. <b>5</b> 5	102.805	43.892	68.483	1.00 89.77	Ċ
MOTA	3706	CB	SER	55	103.373	43.750	69.896	1.00 90.69	Ċ.
MOTA	3707	OG	SER	5 <b>5</b>	102.332	43.662	70.853	1.00 90.09	C
MOTA	3708	C	SER	55 ·	103.617	44.916	67.695	1.00 90.09	C
MOTA	3709	O·	SER	55	103.181	45.378	66.639	1.00 92.24	c
ATOM	3710	N	GLN	56	104.796	45.251	68.218	1.00 90.33	C
ATOM	3711	CA	GLN	56	105.715	46.207	67.600	1.00 93.42	C
MOTA	3712	CB	GLN	56 ·	106.882	45.448	66.957	1.00 94.20	c
MOTA	3713	CG	$G\Gamma N$	56	107.492	44.372	67.861	1.00 94.20	C
MOTA	3714	CD	GLN	· 56	•	43.192	67.088	1.00 99.99	. c
MOTA	3715	OE1	GLN .	56	108.128	42.066	67.595	1.00 87.08	· c
MOTA	3716.	NE2	GLN	56	108.500	43.446	65.854	1.00 95.33	. C
ATOM ·	3717	C	GLN	56	105.040	47.121	66.572	1.00 99.98	C
MOTA	3718	0	GLN	56	104.866	46.744.	65.413		Ċ
MOTA	3719	N	GLN	57	104.670	48.323	67.013 66.177	1.00 83.45	Ċ
MOTA	3720	CA	GLN	57	103.995	49.318		1.00 85.60	c
ATOM .	3721	CB	GLN	. 57	104.417	50.732	66.589 68.084	1.00 89.34	Ċ
ATOM	3722	CG	GLN	57	104.367	50.991	68.718	1.00 87.16	C
ATOM	3723	CD	GLN	57	105.744	50.966	68.635	1.00 76.99	C
ATOM	3724	OEl		57	106.497	51.937	69.355	1.00 90.12	C
ATOM	3725	NE2		· 5 <b>7</b>	106.080	49.849	64.669	1.00 80.35	C
ATOM	3726	C	GLN	5 <b>7</b> ·	104.185	49.175	64.182	1.00 77.96	c
MOTA	3727	.0	GLN	57	105.278	48.877	63.943	1.00 76.47	C
MOTA	3728	N	, LEU	58	103.095	49.401	62.487	1.00 /0.17	Ċ
MOTA	3729	CA	LEU	58	103.077	49.331	61.972	1.00 52.59	, C
MOTA	3730	CB	LEU	. 58 <sub>.</sub>	10.1.723	49.838	60.845	1.00 50.02	Ċ
MOTA	3731	CG	LEU	. 58	. 100.956	49.130	61.070	1.00 55.58	C
MOTA	3732		. LEU	. 58	100.916	47.634	60.794	1.00 39.64	C
MOTA	3733		LEU	58	99.535	49.671	61.906	1.00 54.39	, G
ATOM	3734	C	LEU	58	104.209	50.181 51.345	62.284	1.00 51.09	С
ATOM	3735	0	LEU	58	104.387	.49.589		1.00 51.81	С
ATOM	3736	N	GLN	59 ·	104.976	50.290	60.346	1.00 46.97	С
MOTA	3,737	CA	GLN	59	106.080		60.524		· c
ATOM	37,38	CB	GLN	59	107.394	50.260	61.308	1.00 32.42	С
MOTA	3739	CG	GLN	59	108.469	49.340	62.171	1.00 53.43	C
ATOM	3740	CD	GLN	59.	109.327 110.198	49.799	62.912	1.00 50.95	C
MOTA	3741		L GLN	59 50	109.082	48.037	62.079	1.00 46.72	C
MOTA	3742		2 GLN	59 50	105.748	50.417	58.859	1.00 43.43	C
MOTA	3743	C	GLN	59 59	105.740	49.422	58.138	1.00 42.60	C
MOTA	3744	0	GLN - VAL	· 60	105.505	51.645	58.412	1.00 40.75	C
MOTA	3745			· 60	105.172	51.907	•	1.00 39.80	G.
MOTA	3746		VAL.	60	103.828	52.659	56.896	1.00 26.19	C
MOTA	3747		VAL 1 VAL	60	103.878	53.955	57.678	1.00 21.41	. С
ATOM	3748			60	103.528	52.946	55.448	1.00 27.26	C
ATOM	3749			60	106.267				С
MOTA	3750		VAL	60	106.733			1.00 51.96	. C
ATOM	3751		VAL	. 61	106.692	52.349			C
ATOM	3752		TYR	. 61	107.731			1.00 25.83	C
MOTA	3753			61	109.118				C
ATOM	3754			. 61	109 496				С
MOTA	3755			61	109.216				c
ATOM	. 3756	, (1)			. • •	. '			

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MOTA	3.757	CEl	TYR		61	•	10	9.5	99	48.	819	54	.439	. 3	00	33,	05		C
ATOM	3758	CD2	TYR	٠.	61		1. 11	0.1	L73 ·	· 51.	150	53	.057		L.00				.C
ATOM	3759	CE2	TYR		61		. 11	0.5	662	49.	918	52	. 533	1	.:00	23,	48		C
MOTA	3760	CŻ	TYR		61		11	.0.2	269	48.	758	53	.231	٠ ٦	00	29.	34	•	C
ATOM	3761	ОН	TYR		61	-	11	.0.6	527.	47	535	.52	.714	. 1	00	30.	14		C
MOTA	3762	C	TYR		61		10	7.5	40	52.	981	52	. 986	1	L·. 00	35.	71		C
ATOM	3763	.0	TYR		61		10	6.6	594	52.	214	52	.513	1	00	35.	76		· C
ATOM	3764	N	SER		62	:	10	8.3	122	53.	775	52	.258	1	00	39.	80		, C
MOTA	3765	CA	SER	•	62		10	8.2	268	53.	813	50	.805	1	.00	39.	42		· C
ATOM	3766	CB	SER		62		10	7.2	247	54	857	50	.345	. 1	00	32.	31.		С
ATOM	3767	OG	SER		62		10	7.1	L20	54.	. 853	48	. 932	1	L:00	23.	48		<b>C</b>
MOTA	3768	С	SER		62	•	10	9.6	543	54	.137	50	.220	3	00	45.	43		C
ATOM	3769	ο.	SER		62		11	.0.2	287	55	.116	50	.601	1	.00	42.	20		С
ATOM	3770	N	LYS		63		11	.0.0	94 -	53	.302	49	. 294	1	00	50.	45		C
MOTA	3771	•	LYS		63		11	.1.3	888	53	499	48	. 655	, 3	1.00	44.	30		С
ATOM	3772	·CB	LYS		63	٠.	. 11	2.0	0.40	52	. 136	48	. 373	3	L.00	41.	16		C
ATOM	3773	. CG	LÝS		63		1,1	.3.0	145	51	. 676	49	.431	3	1.00	41.	13		С
ATOM	3774	CD	LYS		б3		11	2.7	720	50	. 288	49	. 969		L.00			•	C
MOTA	3775	CE	LYS.		63		11	.3.7	769	49	. 809	50	. 972	1	L.00	27.	51		C
MOTA	3776	NZ	LYS		63	٠.	11	4.5	917	49	.099		.322		L:00	14.	01		C
ATOM	· 3777 · .	C	LYS		63		. 11	.1.3	173	54	.243	.47	.343	. 1	L.00	40.	39		C
ATOM	3778	Ο.	LYS.	٠.	63		11	20	79	54	.322		.515		L.00	43.	49	•	C
ATOM	3779	N	THR		•64		. 10	9.9	977	.54	. 802	47	.166	.1	1.00	38.	77		C
ATOM '	3780	CA	THR		64	•	10	9.6	535	55	.496	.45	.926	1	1.00	33.	97	•	. C
MOTA	3781	CB	THR		64.		10	8.4	107	54	. 837	.45	.264		1.00				C
ATOM	3782	OG1	THR		64	•	.10	7.4	145	54	. 502	46	. 272	1	1.00	61.	07		. G
MOTA	3783	CG2	THR		64	•	.10	8.8	311	53	.576	44	.520		ι.οο				,C
MOTA	3784	C	THR		64		10	9.3	360	56	.988	. 46	.033	:	1.00	33.	47	•	C
MOTA	3785	0	THR	٠	64		10	9.1	122	57	.651	45	.023	:	1.00	25.	44		C
ATOM	3786	$\cdot \mathbf{N}$	GLY		65,		. 10	9.3	375	57	. 525	47	.244		1.00	35.	21		C
ATOM	3787	CA	GLY	٠	65	•	10	9.3	119	58	. 946	47	.383		1.00	•			; C
ATOM	<b>3788</b>	C	GLY		65	•	10	7 . 6	544	59	. 286		.468		1.00				ĹĠ
ATOM	. 3789	0	GLY		65		10	7.1	198	· 60	.317	46	.970		1.00				C
ATOM	3790	N	PHE		66		10	)6.8	881	58	. 405		.100		1.00				, C
ATOM	3791	CA	PHE		66		. 10	)5.4	454	58	.616	48	.280						C
ATOM	3792	CB	PHE	٠	66		10	)4.6	580	·57	.350	47	.914		1.00				C
ATOM	3793	CG	PHE		66		10	04.3	307	57	. 25_6		.463		1.00				C
ATOM	3794	CD1	DHE.		66		10	05.2	243	56	.859		.514		1.00				C
ATOM	3795	CD2	PHE		66		10	33.0	009		.536		.042		1.00			•	C
ATOM	. 3796	CE1	PHE		66			04.8			.738		.159		1.00				C
ATOM	3797	CE2	PHE.		66	. :	. 10	02.6	648		.419		.694		1.00			•	, C
ATOM	3798	CZ	PHE		66			93.5			.018		.750		1.00				C
ATOM	3799	G.	PHE		66		10	05.2	238		.921				1.00				C
ATOM	3800	0	PHE		66		10	05.	701		.176		.622		1.00				· c
ATOM.	3801	N	ASN.	•	67	•	10	04.	569	60	.028		.053		1.00				C
ATOM	3802	CA	ASN		67		. 10	04.:	289		.375		.436		1.00				С
ATOM	3803	CB	ASN		67				776		:814		.516		1.00				.c
ATOM	3804	CG	asn		67			03.			. 385		.923		1.00				C
ATOM	3805	OD1	ASN		67			03.			.603		.110		1.00			•	C
ATOM	3806	ND2	ASN	•	67			03.1			.507		.922		1.00				C
MOTA	3807	C	ASN		67				208·		.390		.891		1.00			•	·.C
ATOM	3808	Ο.	ASN		67	:		02.			.698		.893		1.00			: '	C
ATOM	3809	N	CYS		68		. 10	03.	627	.58	.190	52	.276	•	1.00				Ċ
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              CB
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MOTA
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                           69
                   ASP
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                                   101.902
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                   ASP
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ATOM
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                                                       58.568
                                              50.274
                                     95.553
                            71
        3835
               0
                    LYS
                                                                                 . C
 ATOM
                                                       60.628
                                                                1.00 51.79
                                              49.940
                                     96.373
                           .72
                    LEU
 МОТА
         3836
               N
                                                                                  C
                                                                1.00 61.74
                                                       60.684
                                              48.564
                                     95.907
                    LEU
                            72
         3837.
               CA
 АТОМ
                                                                                  C
                                                       61.650
                                                                1.00 62.34
                                              47.760
                                     96.773
                    LEU
                            72
               CB
         3838
 ΔΤΟΜ
                                                                                  C
                                                       61.103
                                                                1.00 66.36
                                              46.425
                                     97.284
                            72
               . CG
                    LEU
         3839
 ATOM
                                                                                   C
                                                       62.147
                                                                1.00 68.74
                                              45.754
                                     98.165
                            72
               CD1 LEU
         3840
 ATOM
                                                                                   C
                                                       60.736
                                                                1.00 53.65
                                              45.527
                                     96.107
                            72
                CD2 LEU
 MOTA
         3841
                                                                                   C
                                                       61.090
                                                                1.00 73.73
                                              48.447
                                     94.436
                C
                    LEU
                            72
         3842
 MOTA
                                                                                   C
                                                                1.00 88.59
                                                       61.663
                                     93.860
                                              49.374
                            72
         3843
                0
                    LEU
                                                                                   C
 MOTA
                                                                1.00 67.09
                                              47.298
                                                       60.789
                                     93.835
                            73
                    GLY
         3844
                N
                                                                                   C
 ATOM
                                                               . 1.00 50.60
                                                       61.126
                                              47.075
                                     92:443
                            73
                    GLY
         3845
                CA
 ATOM
                                                                                   C
                                                                1.00 56.73
                                                       60.808
                                              45.670
                                     91.964
                            73
                                                                                   Ç
                C
                    GLY
         3846
 MOTA
                                                                1.00 64.99
                                                       .59.760
                                     91.356
                                              45,434
                            73
                0
                    GLY
         3847
                                                                                   C
 MOTA
                                                                 1.00 46.04
                                                        61.713
                                               44.735
                                     92.246
                            74
                    ASN
         ·3848
                N-
                                                                                   C
 ATOM
                                                                 1.00 54.16
                                                        61.566
                                     91.828
                                               43.342
                            74
                    ASN
                CA
 MOTA
         3849
                                                                                   C
                                                                 1.00 79.65
                                                        61.790
                                               43.231
                                      90.316
                    ASN
         3850
                CB
 ATOM
                                                                                   C
                                                                1.00 90.87
                                                        62.814
                                      89.953
                                               42.174
                             74
                     ASN
         3851
                CG
 ATOM
                                                                                   C
                                                        63.574
                                                                 1.00 90.68
                                      88.992
                                               42.334
                             74
         3852
                OD1
                    ASN
 ATOM
                                                                 1,00 89.35
                                                                                   C
                                                        62.838.
                                      90.715 .41.086
                             74
                ND2 ASN
 MOTA
         3853
                                                                                   C
                                                                 1.00 54.40
                                                        60.215
                                               42.738
                                      92.180
                             74
                     ASN
                C
         3854
 ATOM
                                                                 1.00 62.07
                                                                                   C
                                                        59.951
                                      93.332
                                               42.413
                             74
                     ASN
                0
          3855
  ATOM
                                                                 1.00 55.88
                                                                                   С
                                                        59.364
                                               42.577
                                      91.171
                             75
                     GLU
                N
          3856
                                                                 1.00 47.09
  ATOM
                                                                                   C
                                                        58.035
                                               42.010
                             75
                                      91.364
                     GLU
          3857
                 CA
                                                                                   C
  MOTA
                                                                 1.00 56.56
                                               40.988
                                                        57.722
                                      90.269
                             75
                     GLU
          3858
                                                                                    C
  ATOM
                                                        58.471 . 1.00 48.68
                                               41.211
                                      88.966
                             75
                 CG
                     GLU
          3859
                                                                                    C
  ATOM
                                                        59.379
                                                                 1.00 58.55
                                      88.614
                                               40.047
                             75
                     GLU
          3860
                 CD
  ATOM .
                                                                                    C
                                                                 1.00 55.16
                                                        58.859
                                               38.928
                                      88.407
                             75
                 OE1 GLU
  MOTA
          3861
                                                        60.612
                                                                 1.00 54.08
                                      88.547
                                                40.250
                 OE2 GLU
                             75
          3862
  ATOM
```

				•		7.013	1.00 44.01	С.
ATOM	3863	GLU	75 ·				1.00 27.15	С
ATOM	3864	GLU .	75	20.00	•		1.00 36.46	С
ATOM	3865 h	SER	76				1.00 31.85	С
ATOM		A SER	76	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		6.376	1.00 34.92	С
ATOM		CB SER	76			6.492	1.00 16.45	C
ATOM		G SER	76 .			7.681	1.00 32.47	Ċ
ATOM		SER	76			6.733	1.00 34.00	Ċ
ATOM		SER	76			7.892	1.00 34.00	Ċ
ATOM	3871	VAL	77	93.826	-	55.723	1.00 32.38	Ċ
ATOM		CA VAL	77 .	94.906		55.908	1.00 32.30	Ċ
ATOM		CB VAL	· 77	96.272		55:386	1.00 43.71	Ċ
		CĠ1 VAL	77	96.747		54.190	1.00 37.47	Ċ
MOTA		CG2 VAL	77	97.327		56.484		Ċ
ATOM	• • • •	C VAL	77	94.509		55.101	1.00 33.67	. c
ATOM		O VAL	77 .	93.934		54.013	1.00 38.06	C
ATOM	•.•.	N THR	78	94.811		55.630	1.00 40.03	C
MOTA		CA THR	78	94.475		54.929	1.00 38.24	. c
MOTA	3879	CB THR	78	93.548		55.787	1.00 35.10	. c
ATOM	3880	OG1 THR	78	92.594		56.472	1.00 36.53	
ATOM	3881	CG2 THR	78	92.804		54.916	1.00 36.45	c
ATOM	3882		78	95.745	52.269	54.580	1.00 35.91	
MOTA	3883	-	78	96.574		55.451	1.00 31.92	. C
MOTA	3884		79.	95.896	52.610	53.301	1.00 39.13	C
MOTA	. 3885	•	79 79	97.059	53.358	52.824	1.00 29.89	C
MOTA	3886		79	97.532	52.801	51.487	1.00 35.47	C
MOTA	3887		79 .	97.996	51.380	51.553	1.00 41.67	. C
MOTA	3888		79 . 79	97.174	50.342	51.123	1.00 46.33	, c
MOTA	3889	CD1 PHE	. 79	99,271	51.077	52.019	1.00 35.39	C
MOTA	3890	CD2 PHE	79	97.621	49.026	51.155	1.00 34.72	C
ATOM	3891	CE1 PHE	79	99.724	49.765	52.054	1.00 17.78	C
MOTA	3892	CE2 PHE	. 79	98.895	48.736	51.619	1.00 26.82	C
ATOM	3893	CZ PHE	. 79 79	96.687	54.816	52.645	1.00 20.01	C
ATOM	3894	C PHE	· 79	95.843	55.143	51.817	1.00 39.07	C
MOTA	3895	O PHE	80	97.328	55.690	53.414	1.00 37.92	. c
MOTA	3896	N TYR	80	97.048	57.123	53.361	1.00 39.66	C
MOTA	3897	CA TYR	80	97.043	57.706	54.775	1.00 41.42	٦٠
MOTA	3898	CB TYR	80	96.541		54.849	1.00 29.87	C
ATOM.	3899	CG TYR	80.	95.857		53.782	1.00 31.82	С
ATOM	3900	CD1 TYR		.95.404		53.842	1.00 38.26	C
MOTA	3901	CE1 TYR	80 80	96.756		55.984	1.00 35.48	C
MOTA	3902	CD2 TYR		96.307		56.060	1.00 38.78	, C
ATOM	3903	CE2 TYR	80	95.632		.54.984	1.00 46.52	C
MOTA		CZ TYR	. 80 80	95.195		55.046	1.00 43.37	. C
ATOM		OH TYR	_	98.034		52.508	3 1.00 36.43	· C
MOTA		C TYR	80 80	98.960		53.028	1.00 41.51	C
ATOM		O TYR	81	97.817		51.199	1.00 37.66	C
MOTA		N LEU	81	. 98.694		50.26	3 · 1.00 43.35	C
ATOM		CA LEU		98.538		48.86	1 1.00 40.97	C
ATOM		CB LEU	· 81	98.392		48.72	1 1.00 35.20	
ATOM			81	98.068		47.26	B 1.00 41.59	Ċ
ATOM			81	99.67		49.14	1 1.00 34.03	C
ATOM			81	98, 45	<del>-</del>		6 1.00 39.41	C
MOTA				97.41				С
ATOM	4 3915	O LEU	81	J 44.		• • .	•	
					_		·	

				•		CO 053:	50.678	1.00 45.56	C
TOM	3916		GLN	82 .				1.00 47.39	C
MOT	3917	CA	GLN .	82				1.00 48.95	c ·
	3918	CB	GLN	82	99.884			1.00 42.53	· C
TOM	3919	CG ,	GLN	,82	99.479			1,00 35.76	. C
TOM	3920	CD	GLN	82	99.397	62.514		1.00 35.27	С
TOM	3921	OE1	GLN	82	99.826	64.127		1.00 29.92	C
TOM	3922	NE2	GLN	82	98.857	62.884	49.571	1.00 42.88	C
MOT	3923	C	GLN	82	100.280	62.194	49.035	1.00 41.58	· C
TOM	3924	<b>O</b> .	GLN	82	101.148	64.148	49.237	1.00 45,46	C
MOT	3925	N	ASN	83	100.060	64.806	48.197	1.00 43.88	C
MOT	3926	CA	ASN	.83.	100.843		48.748	1.00 38.56	C
TOM	3927	CB	. ASN	83	102.229	66.242	49.779	1.00 47.82	C
MOTA	3928	CG.	ASN	83	102.170	67.083	49.735	1.00 46.58	Ċ
MOT	3929	OD1	ASN	83	101.274	66:249	50.715	1.00 33.98	C
MOTA	3930	ND2	ASN	83	103.118	63.966	46.933	1.00 37.91	· C
MOTA	.3931	C	ASN .	83 ·	100.951		46.424	1.00 45.24	С
MOTA	3932	Ο.	asn	83	102.045	63.535	46.430	1.00 28.03	,C
MOTA	3933	$\cdot$ N	LEU	84	99.803	62.723	45.230	1.00 19.39	C
MOTA	3934	CA	LEU	84	99.760	61.802	45.263	1.00 26.73	. с .
MOTA	3935	CB	LEU	84	98.540 98.774	60.341	45.664	1.00 34.93	С
MOTA	3936	.CG	LEU	84	98.774	59.552	45.502	1.00 37.57	C
MOTA	3937		LEU	84	99.877	59.729	44.812	1.00 36.66	C
MOTA	3938	ÇD2	LEU	84	99.675	63.650	44.037	1.00 20.07	,c
MOTA	3939	С	LEU	84	98.914	64.609	44.049	1.00 31.39	C
MOTA	3940	0	LEU	84 .	100.460	63.365	43.006	1.00 33.90	Ċ
MOTA	3941	N	TYR	85	100.464	64.187	41.806	1.00 40.42	· с
MOTA	3942	CA	_	85	101.840	64.117	41.123	1.00~59.23	C
ATOM	3943	CB		85	102.989	64.613	41.980	1.00 61.79	· C
ATOM	3944	CG		85	103.155	65.973	42.242	1.00 63.76	C
MOTA	3945		1 TYR	85	103.133	66.430	43:053	1.00 67.56	C
ATOM	3946		1 TYR	85	103.897	63.717		1.00 64.22	·C
MOTA	3947	CD		85 .	104.938			1.00 65.83	C
MOTA	.3948			85 85	105.079			1.00 70.24	C
MOTA	3949			85	106.093			1.00 73.68	C
MOTA	3950			85 · 85	99.378			1.00 33.25	C
MOTA	3951		TYR	85	98.880			1.00 33.16	C
MOTA	3952		TYR	85	99.018			1.00 32.80	C
ATOM	3953		VAL	.86 86	97.994	-		1.00 31.92	C
MOTA	3954			86 86	97.503	·	38.241		, с
ATOM.	3955			86	98.476			1.00 32.20	C
MOTA	3956		31 VAL	86 86	97.361		36.743	1:00 34.84	C
MOTA	3957		32 VAL		98.504		37.854		C
MOTA	3958		VAL	86	97.72	•	1 37.204	1:00 28.12	C
ATOM	3959				99.81		37.685	1.00 37.39	C
MOTA	3960			87	100.41		0 36.716	1.00 31.78	C
MOTA	396			87	101.80		1 36.348		C
MOTA	396			87	102.72		6 37.542		C
MOTA					102.33	4 62.46			. C
ATOM			D1 ASN D2 ASN		103.93		0 37.35	1.00 44.07	. C
ATOM					100.50	4 60.95	5 37.37		C
MOTA		_			100.96	4 59.98	1 36.77		C
ATOM					100.06			7 1.00 33.61	
ATOM	396	8 1	, GIIIN	, ,	• .				

•						50 CCE	39.402	1.00 24.73	С
TOM	3969	-	GTM .	88	100.082	59.665 59.983	40.871	1.00 26.06	С.
TOM.	3970		GLN	88	100.430	59.314		1.00 44.43	С
MOT	3971		GLN	88	101.721	60.285	42.081	1.00 36.54	C .
MOT	3972		GLN	88.	102.692	60.675	43.235	1.00 26.99	C
MOT	3973	OEl	GLN	88	102.504	60.668 .		1.00 38.97	. G
MOT	3974	NE2	GLN.	88	103.743	58.896	39.322	1.00 26.16	. с
MOT	3975	C	GLN ·	88	98.747	57.805	39.872	1.00 22.71	, C
MOT	3976	0	GLN	. 88	98.635	59.448	38.645	1.00 29.74	Ċ
MOTA	3977	N	THR	89	97.735	58.742	38.548	1.00 35.51	С
MOTA	3978 .	CA	THR	89	96.450	59.548	37.786	1.00 23.56	, G
MOTA	3979	CB	THR	89	95.381	59.391	36.381	1.00 37.82	С
MOTA	3980	OG1	THR	89	95.586	61.008	38.140	1.00 8.56	C
MOTA	3981	CG2	THR	89	95.456	57.434	37.808	1.00 30.57	C
MOTA	3982	С	THR	89	96.686	57.427	36.701	1.00 19.99	С
MOTA	3983	0	THR .	89	97.222	56.326	38.411	1.00 26.02	, с.
MOTA	3984	N	ASP	90 '	96.274	55.032	37.799	1.00 29.88	Ć c
ATOM .	3985	CA	ASP	90	96.520	54.758	37.848	1.00 17.27	. C
MOTA	3986	CB	ASP	90	98.023	53.857	36.738	1.00 29.31	Ċ
MOTA	3987	CG	ASP	90	98.492 99.661	54.010	36.312	1.00 28.02	. C
ATOM	3988		ASP	90 .	= "	53.002	36.299	1.00 35.12	С
MOTA	3989		ASP	. 90	97.695 95.774	53.918	38.519	1.00 32.73	C
MOTA	3990	С	ASP	90	94.869	54.181	39.307	1.00 28.33	. C
MOTA	3991	0	ASP	90	96.155	52.674	38.234	1.00 33.15	C
MOTA	3992	N	ILE	91	95.549	51.524	38.891	1.00 29.34	, <b>C</b>
MOTA	. 3993	CA	ILE	91	95.320	50:330		1.00 19.19	C
MOTA	3994	CB	ILE	91	93.891	49.803	38.124	1.00 7.46	С
MOTA	3995	CG2		91	95.613	50.734	36.525	1.00 24.90	C
MOTA	3996	CG1		91	96.736	49.967	35.904		C.
MOTA	3997	CD1		91	96.539	51.070	39.929	1.00 33.79	C
MOTA	3998	·C	ILE	91	97.707	50.844	39.615	1.00 35.59	C
MOTA	3999	0	ILE	91 : 92	96.064	50.948	41.162	1.00 39.40	C
MOTA	4000	N	TYR	92	96.891	50.521	42.274	1.00 25.36	C
ATOM	4001	CA	TYR	92	96.817	51.555	43.398	1.00 24.66	C
MOTA	4002	CB	TYR	92 . 92	97.472	52.872	43.039		С
MOTA	4003	.CG	TYR	92	98.646	53.282	43.669	1.00 32.14	С
MOTA	4004	CD:		92	99.265			1.00 24.99	С
MOTA	4005			92 92	96.933	53.697			· C
MOTA	4006			92	97.547			1.00 24.44	. с
MOTA	4007			92	98.712	·			C
MOTA	4008		•	92	99.332		42.010		C
MOTA	4009		TYR	92	96.381	_	42.761		Ċ
MOTA	4010		TYR	92	95.173		42.791	1.00 36.33	C
ATOM	4011			93.	97.303		43.127	1.00 28.40	C
MOTA	4012		PHE PHE	93	96.931		43.621	1.00 29.94	C
ATOM	4013			93	97.448		42.689		. C
MOTA	4014			93	97.105			1.00 24.43	
MOTA	4015		1 PHE	93	97.978		3 40.422		C
MOTA	4016		2 PHE		95.92		7 40.733	1.00 30.96	C
ATOM	4017		1 PHE	93	97.673		3 39.076	1.00 46.97	C
ATOM	4018			93	95.61		2 3939		. C
MOTA	4019 4029			93	96.483	3 46.46	7 38.562		C
ATOM	402		PHE	93	97.47		9 45.020	1.00 35.26	,C
MOTA	404.	_ `	~ ~~~	٠,			•	•	• '

	•	•				47.022	45.325	1.00 34.73	C
MOT	4022	ο .	PHE	93	98.635	46.209	45.870	1.00 48.06	Ċ
MOTA	4023	И	CYS	94	96.601	45.907	47.235	1.00 36.83	. С
MOTA	4024	CA	CYS	94	96.969	44,546	47.284	1.00 31.31	C
MOTA	4025	C	CYS	94	97.635	43.692	46.431	1.00 33.02	C
ATOM	4026	ο .	CYS	94	97.397	45.921	48.121	1.00 39.16	C .
ATOM	4027	CB	CAR	94	95.738	46.711	49.706	1.00 59.22	C
ATOM	4028	SG	CYS	94	96.102	44.349	48.288	1.00 35.15	С
ATOM	4029	N	LYS	95	98.475		48.430	1.00 32.02	C
MOTA	4030	CA	LYS	.95	99.194	43.033	47.824	1.00 20.95	С
MOTA	4031	CB	LYS	95	100.593	41.913		1.00 16.51	С
· MOTA	4032	CG	LYS ·	95	101.265		47.179	1.00 20.20	С
ATOM	4033	CD	LYS	95	. 102.720	42.111 40.772	46.979	1.00 39.20	С
ATOM	4034	CE	LYS	95	103.419		46.471	1.00 47.09	. C
atom	4035	NZ	LYS	.95	104.812	42.731	49.896		C ·
MOTA	4036	C.	LYS	95	99.301	42.731	50.759	1.00 32.79	. <b>C</b>
MOTA	4037	0	LYS	95	99.224	41.444	50.172	1.00 24.46	C
MOTA	4038	И	ILE	96	99.480	40.978	51.542	1.00 19.72	C
MOTA	4039		ILE	96.	99.619	40.925	52.251	1.00 14.76	C
ATOM	4040	CB	ILE	96	98.258	40.052	51.477	1.00 17.83	·C
ATOM	4041	CG2		96	97.299	40.405	53.673	1.00 17.25	C
atom	4042	CG1		96	- 98.434	41.352	54.570	1.00 5.02	C
ATOM.	. 4043	CD1		96	99.184	39.599	51.602	1.00 26.57	С
ATOM	4044	C ·	ILE	96	100.276	38.662	50.916	1.00 34.37	C
ATOM	4045	0	ILE	96	99.852	39.491	52.419	1.00 20.47	С
MOTA	4046	N	GLU	97 `	101.321	38.243	52.592	1.00 27.23	C
ATOM	4047	CA	GLU	97	102.052	38.279		1.00 32.57	C
МОТА	4048	CB	GLU	97	103.367	39.550	51.949	1.00 38.60	C.
MOTA	4049	CG	GLU	97	104.186 104.535	40.193	50.618	1.00 46.08	C
ATOM	4050	CD		97	105.239	39.548	49.815	1.00 37.73	C "
ATOM	4051		l GLU	97	104.108	41.348	50.379	1.00 54.19	.C
ATOM	4052	OE:		97 97	102.343	37.951	54.071	1.00 30.22	C
ATOM	4053	.C	GLU	97	102.705	38.841		1.00 27.30	C
ATOM	4054	.0	GLU	. 98	102.158	36.694	54.455		С
MOTA	4055	N	VAL.	98	102.395		55.817	1.00 17.97	. С
ATOM	4056			98•	101.361	35.183		1.00 33.66	C.
ATOM	4057		VAL 1 VAL	98	102.002			1.00 46.61	C.
ATOM	4058		2 VAL	98	100.200			1.00 31.46	c.
MOTA	4059		VAL	_	103.787		55.808		C
MOTA	4060		LAV	98	104.147		54.858		C.
ATOM	4061		MET	99	104.569		56.851		C
ATOM	4062			99	105.932		56.940		c
ATOM	4 0.63			99	106.951	_	56.753	1.00 26.44	,C
MOTA	4064		·	99	106.449				, C
MOTA				99	106.981		56.039	1.00 49.54	C
ATOM	4066			99	105.587				C
ATOM	4067		MET	∵ 99	106.182		58.273		C
ATOM	4068		MET	99	107.286				C
ATOM			TYR	100	105.154		59.119	<b>-</b>	C
ATOM				100	105.210	34.084			, с
ATOM				100	106.44				· C
MOTA				100	106.97				. С
MOTA			D1 TYR	100	107.90	8 32.54	61.74	5. 1.00 66.10	. С
ATOM	. +0/						•		•

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C
                                                              1.00 67.96
                                                    62.622
                                            31.625
                                  108.466
                         100
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              CE1
       4075
MOTA
                                                              1.00 50.84
                                            33.483
                                                     63.. 523
                                 . 106.611
                         100
              CD2
                                                                                C
MOTA
       407.6
                                                              1.00 57.94.
                                            32.559
                                                     64.415
                                  107.166
                         100
                  TYR
MOTA
       4077
              CE2
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                                                              1.00 57.97
                                            31.636
                                                     63.951
                                  108.098
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                  TYR
             ·CZ
MOTA
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                                                              1.00 53.54
                                            30.728
                                                     64.801
                                  108.687
                         100
                  TYR
              OH
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MOTA
       4079
                                                              1.00 49.53
                                                     61.259
                                            34.429
                                  103.978
                         100
                   TYR
              C
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ATOM
       4080
                                                              1.00 42.87
                                                     61.307
                                            35.587
                                  103.561
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              ο.
                   TYR
                                                                                C
       4081
ATOM
                                                              1.00 53.02
                                                     61.920
                                            33.422
                                  103.380
                         .101
                   PRO
       4082
              N
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MOTA
                                                     62.771
                                                              1.00 52.41
                                            33.528
                                  102.180
                         101
                   PRO
       4083
              CD
                                                              1.00 46.66
MOTA
                                                     61.844
                                            32.054
                                  103.902
                   PRO
                         101
              CA
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       4084
MOTA
                                                     62.927
                                                              1.00 42.16
                                            31.300
                                  103.126
                         101
              CB
                   PRO
       4085
MOTA
                                                     63.189
                                                              1.00 38.19
                                  101.906
                                             32.115
                         101
                   PRO
        4086
              CG
atom
                                                              1.00 57.32
                                                      60.441
                                  103.711
                                             31.468
                          101
                   PRO
        4087
              C .
                                                              1.00 47.74
MOTA
                                                      59.648
                                  .102.901
                                             31.960
                          101
                   PRO
        4088
              0
ATOM
                                                    .60.122:
                                                              1.00 58.81
                                  104.455
                                             30:400
                   PRO
                          102
        4089 .
              N.
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                                                               1.00 43.99
MOTA
                                                      61.000
                                             29.707
                                   105.410
                          102
                   PRO
              CD
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        4090
                                                               1.00 54.29
MOTA
                                             29.758
                                                      58.807
                                   104.368
                          102
                   PRO
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        4091
               CA
                                                      58.766 1.00 46.96
MOTA
                                             28.824
                                  105.585
                          102
                   PRO
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               CB
                                                               1.00 46.28
MOTA
        4092
                                   106.354 29.090
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                   PRO
                          102
                                                                                 C
               CG
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                                                               1.00 50.83
MOTA
                                                      58.565
                                             28.997
                                  .103.072
               C
                   PRO
                          102
                                                                                 C
                                                               1.00.51.79
        4094
ATOM
                                             28.812
                                                      59.475
                                   102.265
                          102
        4095
               0
                   PRO
                                                                                 C
                                                               1.00 43.58
ATOM
                                                      57.321
                                             28.550
                                   102.858
                          103
              N
                   PRO
                                                                                 C
        4096
                                                               1.00 38.84
MOTA
                                             27.757
                                                      56.901
                                   101.692
                          103
                   PRO
               CD
                                                                                 C
MOTA
        4097
                                                               1.00 34.80
                                                      56.209
                                             28.756
                                   103.784
                   PRO
                          103
               CA
                                                                                 C
        4098
                                                               1.00 35.84
ATOM
                                             27.611
                                                      55.247
                                   103.457
                          103
               CB
                    PRO
                                                                                 C
        4099
 MOTA
                                                               1.00 31.11
                                                      55.860
                                             26.863
                                   102.280
                          103
                    PRO
         4100
               CG
                                                                                 C
                                                               1.00 39.20
 ATOM
                                                      55.566
                                             30.127
                                   103.581
                          103
         4101
                    PRO
                                                                                 C
               C
                                                               1.00 35.30
 MOTA
                                                      56:055
                                             30.939
                                   102.790
                           103
        4102
                    PRO
                                                                                 C
               0
                                                              1.00 40.51
 MOTA
                                                      54.481
                                              30.382
                                   104.311
                           104
               N
                    TYR
                                                                                 C
         4103
                                                               1.00.40.50
 MOTA
                                                      53.760
                                              31.644
                                   104.199
                           104
         4104
               ·CA
                    TYR
                                                                                  C
                                                               1.00 34.12
 MOTA
                                                       52.630
                                              31.719
                                   105.226
                           104
                CB
                    TYR
                                                                                  C
         4105
                                                                1.00 35.99
 MOTA
                                                       51.888
                                              33.036
                                   105.224
                           104
                   ·TYR
                                                                                  C
         4106
                CG-
                                                               1.00 49.18
 ATOM
                                                       50.615
                                    104.659
                                              33.143
                          .104
                CD1 TYR
                                                               1.00 50.34
                                                                                  C
 АТОМ
         4107
                                                       49.926
                                              34.363
                                    104.652
                           104
                CEL TYR
                                                                1.00 34.98
                                                                                  C
         4108
 ATOM
                                              34.179
                                                       52.458
                                    105.784
                           104
                                                               1.00 35.62
                    TYR
                                                                                  C
         4109
                CD2
                                    105.782. 35.403 . 51.779
 МОТА
                           104
                    TYR
                                                                                  C
                CE2
                                                       50.518 1.00 39.99
 MOTA
         4110
                                              35.485
                                    105.215
                           104
                    TYR
                                                                                  C
                CZ
                                                               1.00 32.85
         4111
 ATOM
                                  105.205 36.685
                                                       49.853
                           104
                    TYR
         4112
               . OH
                                                                                  C
                                                                1.00 44.36
 ATOM
                                                       53.168
                                              31.725
                                    102.804
                           .104
                C
                     TYR
         4113
                                                       52.603
                                                                1.00 46.76
 ATOM
                                    102.311
                                              30.749
                           104
                     TYR
                                                                                  C
         4114
                O
 MOTA
                                                                1.00 47 99
                                                       53.304
                                    102.171
                                              32.885
                           105
                     LEU
                                                                                  C
         4115
                N
                                                                1.00 43.06
  ATOM
                                                       52.778
                                               33.096
                                    100.827
                           105
                     LEU
                                                                1.00 44.75
                                                                                   C
         4116
                CA
  MOTA
                                                       53.929
                                               33.347
                                     99.859
                           105
                     LEU
                                                                                   C
         4117
                CB
                                                                1.00 55.87
  MOTA
                                                       54.097
                                               32.310
                                      98.748
                     LEU
                           105
                                                                                   C
                CG ·
                                                                1.00 60.46
          4118
  MOTA
                                                       52.725
                                               31.958
                                     98.181
                            105
                                                                                   C
                CD1 LEU
                                                                1.00 56.52
          4119
                                               31.062 54.797
  MOTA
                                     99.289
                            105
                 CD2 LEU
                                                                                   C
          4120
                                                                 1.00 45.31
  ATOM
                                               34.283 51.813
                                     100.819
                            105
                 C
                     LEU
                                                                                   C
          4121
                                                                 1.00 44.10
                                                        52:085
  MOTA
                                               35.308
                                     101:438
                            105 .
                     LEU
                                                                                   C
                 0
          4122
                                                                 1.00 53.21
  ATOM
                                                        50.696
                                               34.144
                                     100.107
                    ASP
                            106
                                                                                   C
                 N
          4123
                                                                 1.00 56.65
  ATOM
                                               35.199
                                                        49.681
                                     100.046
                            106
                 CA: ASP
                                                                 1.00 73.34
          4124
  MOTA
                                                        48.512
                                               34.827
                            106
                                     100.961
                 CB . ASP
                                                                 1.00 81.75
          4125
                                                        47.979
  ATOM
                                               36.011
                                     101.724
                            106
                 CG ASP
                                                                 1.00 85.62
          4126
  MOTA
                                                        48.432
                                     101.437
                                               37.143
                            106
                 OD1 ASP
         . 4127
  MOTA
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•						•		4 100	1.00 80	) 61		C
TOM	4128	OD2	ASP	106	•	102.603	35.802		1.00 5			·C
TOM	4129	C	ASP	106	•	98.639	35.462		1.00 6			Ċ.
TOM .	4130	0	ASP	106		97.772	34.592	49.199 48.609	1.00 4			C.
TOM	4131	N·	asn	107		98.422	36.658					C
TOM	4132	CA	ASN	107		97.110	37.028		1.00 4			С
TOM	4133	CB	asn	107		96.826			1.00 4			C .
TOM	4134	CG	ASN	107		97.855	39.393	47.736 46.607	1.00 4			С
TOM	4135	OD1	ASN	107	•	97.691	39.852	48.461	1.00 3			С
TOM	4136	ND2	ASN	107	•	98.940	39.637	46.564	1.00 5			C
TOM	4137	C	asn	107		96.997	36.815		1.00 5			С
TOM	4138	0	asn	107		97.990	36.865	46.098	1.00 6		•	C
· MOTA	4139	N	GLU	108 .		95.771	36.601	44.678	1.00 6			С
MOTA	4140	CA	GLU.	108 .	Ċ	95.513	36.393	44.485	1.00 6			С
MOTA	4141	CB	GĽÚ	108 .		94.305	35.474	45.757	1.00 7			C
MOTA	4142	CG	GLU	108.		93.817	34.809	46.180	1.00 7			Ċ
MOTA	4143	CD	GŁU	108			35.295	46.327	1.00 5			C .
MOTA	4144	OE1	GLU ·	108	•	91.534	34:453		1.00 7		•	С
	4145	OE2	GLU	108··		92.285	36.522	43.991	1.00			C
ATOM ATOM ATOM ATOM	4146	C	GLU	108			37.722	43.936	1.00		•	C ·
ATOM.	4147	0	GLU	. 108		94.094	38.171	43.467	1.00			Ċ
MOTA	4148	. N	rys	109		96.306	38.339 39.629	42.782	1.00			С
MOTA	4149	CA	LYS	109		96.215	39.629	41.274	1.00		•	С
MOTA MOTA MOTA	4150	СВ	LYS	109		96.054	39.420	40.666	1.00	66.29		C
MOTA	4151	CG	LYS	109		97.094	39.235	40.373	1.00			, C
MOTA	4152	CD.	••	109		98.399		39.432	1.00			С
MOTA	4153	CE	LYS			99.309			1.00	53.39		Ċ
MOTA			LYS	109	•	100.234		43.331	1.00	59.47		. C
MOTA	4155	C	LYS	109		95.040 94.893		44.545	1.00	73.09		· C
MOTA	4156	0	LYS	109		94.201		42.440	1.00			C
MOTA	4157	'N	SER	110		93.038				50.60		С
MOTA	4158			110		93.404				48.38		С
MOTA	4159			110	•	93.807			.1.00.			C
MOTA	4160			110		92.455	•			49.16		С
ATOM	4161		SER	110 110		93.098				36.85	•	C.
ATOM.	4162		SER	111		91.228				50.24		C.
MOTA	4163		ASN			90.580				48.26		C
MOTA	4164			111 111		89.073			1.00	50.05	:	C
MOTA	4165			111		88.27	<b></b>			52.55		C
MOTA	4166	••	ASN ASN	.111		87.10		40.671		30.90		C
MOTA	4167		OZ ASN	111		88.91		39.413		60.36		C.
ATOM '	4168		ASN			91.21	•	40.708		42.47	•	· C
ATOM	4169		~ ~			90.98	2 45.896	5 <sup>.</sup> 39.748		48.01		C
ATOM	4170		ASN GLY	•		92.00	7 45:517	7 41.717		44.01		C
ATOM						92.68	2 46.808			36.00		. C
ATOM	4173		GLY			91.83		5 42.08		36.58		. C
ATOM.			GLY		٠.	90.63	0 47.89	2 42.343	1.00	33.31		: C
MOTA						92.45		9 42.094		28.16		. C
MOŢA					•	91.73	8 50.41	6 42.403		29.29		
MOTA		7 . C				91.67	1 50.66			25.84		c
ATOM			G1 THE	·		90.95	9 51.88			13.15		c
MOTA			G2 THE			93.06	1 50.76			35.81 29.94		. c
ATOM		_				92.34	4 51.63	6 41.72	2 1.00	43.34	•	<u> </u>
MOTA								· , •		•		٠.

						-0 7-7	42.133	1.00 21.21	. C
MOT.	4181	0	THR	113	93.375		40.662	1.00 31.79	C
MOT	4182	N	ILE	114	91.679	52.074 53.243	39.905	1.00 24.64	C
MOT	4183	CA	ILE	114.	92.093	53.243	38.721	1.00 29.78	. c
MOTA	4184	CB	ILE	114	91.132		38.361	1.00 29.89	· c
MOTA	4185	CG2	ILE	114	91.159	55.001	37.519	1.00 45.18	С
MOTA	4186	CG1	ILE	114	91.510	52.661	36.182	1.00 48.49	C
MOTA	4187	CD1	ILE	114	91.376	53.376	40.821	1.00 21.71	C·
MOTA	4188	С	ILE	114	92.019	54.450	41.546	1.00 23.04	C
MOTA	4189	.0	ILE	114	91.050	54.632	40.770	1.00 22.63	C
MOTA	4190	N	ILE	115	93.028	55.296	41.593	1.00 25.37	C
MOTA	4191	CA	ILE	115	93.003	56.483	42.585	1.00 19.98	C
MOTA	4192	CB	ILE	115	94.147	56.461	42.303	1.00 15.47	c
MOTA	4193	CG2	ILE	115	94.249	57.798	43.558	1.00 5.93	C
MOTA	4194	CG1	ILE	115	93.925	55.312	44.508	1.00 25.93	· c
MOTA	4195	CD1	ILE	115	95.089	55.086	40.701	1.00 36.88	Ċ
MOTA	4196	C·	ILE	. 115	93.104	57.712		1.00 39.31	C
ATOM	4197	0	ILE	115	94.147	57.984	40.112	1.00 36.64	Ċ.
ATOM	4198	N	HIS	116	92.003	58.445	40.604	1.00 42.31	C
MOTA	4199	CA	HIS	116	91.951	59.641	39.779	1.00 42.51	c
MOTA	4200	CB	HIS	. 116	90.530	.59.854	39.250	1.00 53.01	.c
ATOM	4201	CG	HIS	116.	90.397	61.008	38.303	1.00 53.01	Ċ.
MOTA	4202	CD2	HIS	116	. 89.311	61.534	37.690	1.00 33.33	Ċ
MOTA	4203		HIS	116	91.473	61.764	37.884		· c
MOTA	4204		HIS	116	91.054	62.700	37.058	1.00 46.03	· c
ATOM	4205		HIS	116	89.744	62.584	36.920	1.00 38.13	Ċ
MOTA	4206	С	HIS	116	92.380	60.847	40.592	1.00 35.13	· c
ATOM	4207	. 0	HIS	116	91.655	61.278	41.486	1.00 35.30	Ċ.
ATOM	4208	N	VAL.	117	93.554	61.387	40.274	1.00 35.30	c
ATOM	4209	CA	VAL	117	94.078	62.550	40.980	1.00 36.01	, c
ATOM	4210	·CB	VAL	117	95.606		41.146		Ċ
ATOM	4211	CG:	L VAL	117	96.075				Ċ
ATOM	4212			117	96.004				Ċ.
MOTA	4213		VAL	117	93.747				C
ATOM	4214	_	. VAL	117	93.901	63.973			Ċ.
ATOM	4215		LYS	118	93.304				Ċ
ATOM	4216		LYS	118	92.926				Ċ
ATOM	4217		LYS	118	94.076				C
ATOM	4218		LYS	118	94.137				c
ATOM	4219			118	93.956		•		Ċ
ATOM	4220			118	94.163				. c
MOTA	4221			118	95.564				· c
MOTA	4222		LYS	118	. 91.693				C
ATOM	4223		LYS	118	91.566				
MOTA	4224			118	90.87	2 65.178	3 39.832		
END								• •	

#### <u> Fable 5</u>

#### DNA sequence of human CD28 cDNA

				cacacttcgg	attecteggg	60
agactctcag	gccttggcag	gtgcgtcttt	cagccccccc	cacacttegg	actettaget	120
						180
						240
						300
		ACETCACAAA.	duat tagas	3-33		360
						420
						480
						540
						600
						660
						720
						780
						840
						900
						960
						1020 .
						1080
						1140
						1200
						1260
						1320
						1380
						1440
ccaaatgagg	gatteggtes	atgagactto	agtgttaatg	g ttcacaatat	actitcgaaa	1500
tgctttcctc	accectgu	. 46545466		_		1514.
gaataaaata	gccc				*	

## Amino acid sequence of human CD28 (SEQ ID NO:1)

MLRLLLALNL FPSIQVTGNK ILVKQSPMLV AYDNAVNLSC KYSYNLFSRE FRASLHKGLD SAVEVCVVYG NYSQQLQVYS KTGFNCDGKL GNESVTFYLQ NLYVNQTDIY FCKIEVMYPP PYLDNEKSNG TIIHVKGKHL CPSPLFPGPS KPFWVLVVVG GVLACYSLLV TVAFIIFWVR SKRSRLLHSD YMNMTPRRPG PTRKHYQPYA PPRDFAAYRS

The extracellular domain is shown in bold The stalk region is underlined

#### Table 6

### CD28TFc sequence (SEQ ID NO:2)

(thrombin site separating the two halves of the chimera is shown in bold)

•							•		•		•		•									
	CCC	CAT	rcco	3CT(	CAAC	CAG	GCC	CACC	CATO	3GA'	rtg:	GCT	GCG(	GAA	CTT	GCT	ATT +	CCT	GAT	GGCG	60	
. 1	GGG	CTZ	AGG(	CGAC	3TTC	CGTO	CGC	<b>JTG</b> (	ATE	CCT	AAC	CGA	CGC	CTT	GAA	CGA	TAA	GGA	.CTA	CCGC		
	GĢC					•	•		М	D.			·R			L.				A	-	
•						•	•						٠.									
	GC	CGC'	rca.	AAG'	TAT	CAA	CGC	GAA	CAA	GAT	CTT	GGT	'GAA	GCA	GTC	GCC	CAT	'GC'I	"TG1	AGCG	120	
61			 7 (2171)	-+- 	 ልሞል	 GTT(	+ GCG(	 CTT	 GTT	 CTA	GAA	CCA	CTT	CGT	CAG	CGG	GTA	CGF	LAC#	TCGC	•	
•	CGG							•			•		ĸ			P	M		v		<b>-</b> .	
	A	À	Q	,S	I	Ŋ	A	N	K	Τ.		٧.	K	. *	٠		,					
•	• •		٠,			· .	· , .		amo	תאס	C TO TO	· ጥጥር	ነር ጥ	CAA	TCI	CTI	CTC	AA.	3GG2	GTTC	!	
121	TA	CGA	CAA	TGC.	GGT	CAA	+ CCI	TAG			+			-+-				·		+	180	
121	TACGACAATGCGGTCAACCTTAGCTGCAAGTATTCCTACAATCTCTTCTCAAGGGAGTTC  ATGCTGTTACGCCAGTTGGAATCGACGTTCATAAGGATGTTAGAGAAGAGTTCCCTCAAG  Y D N A V N L S C K Y S Y N L F S R E F																					
	· V	D	N	· A	v	· N	L	s	C	K	Y	s	Y	N	L.	, F	S	R	E	F	-	
•	_			-	. •			•				•				•						
	CG	GGC	'ATC	CCI	TCA	CAA	AGG	ACI	GGF	ATA	FTG(	CTG'	rgg/	\AG	rct	GTG:	rtg'	TAT.	ATG	GGAAT 	240	
181				-+-				 ייניטייי		 የውጥረ	- + - ·	GAC	ACC	+ · rtc/	AGA	CAC	AAC	ATA	TAC	CCTTA	4	
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AGNTFTCSVLHEGLHNHHTE

AAGAGCCTCTCCCACTCTCCTGGTAAATAA

1141 ----+ 1170
TTCTCGGAGAGGGGTGAGAGGACCATTTATT

KSLSHSPGK\*

#### **CLAIMS**

- 1. Method of identifying a modulator of CD28 comprising comparing a structural model of a candidate modulator with a structural model of CD28 to thereby determine whether the modulator will bind to CD28, wherein the structural model is derived from, or comprises, structural coordinates of a crystal of: (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii).
- 2. Method according to claim 1 wherein said comparison comprises fitting (docking) the structural model of the candidate modulator with the structural model of CD28, and optionally determining the binding free energy of binding between the candidate modulator and CD28, wherein a low (more negative) binding free energy indicates that the candidate is likely to bind to CD28.

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- 3. Method according to claim 2 wherein the binding free energy is calculated by
  (i) summing the free energies of interatomic contacts between the structural model of
  the candidate modulator and the structural model of CD28, or
  (ii) determining the free binding energy between the force field of the candidate
  modulator and the force field of CD28.
- 4. Method according to any one of the preceding claims wherein whether or not the candidate modulator binds to CD28 comprises comparing the fitting of the structural model of the candidate modulator and the structural model of CD28 with the fitting of a structural model of another protein bound to a ligand, to thereby determine whether or not the candidate modulator will bind to CD28.
- 5. Use of the structural coordinates of a crystal of (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii), to identify a modulator of CD28.
- 6. Method or use according to any one of the preceding claims wherein the structural coordinates are obtainable by subjecting a crystal of (i) CD28, (ii) a

fragment of CD28, or (iii) a homologue of (i) or (ii), to X-ray diffraction measurements and deducing the structural coordinates from the diffraction measurements.

- 7. Method or use according to any one of the preceding claims wherein the crystal is of (i), (ii) or (iii) bound to a CD28 specific antibody or a fragment of said antibody.
- 8. Method or use according to any one of the preceding claims wherein the crystal has the structural coordinates shown in Table 4.
  - 9. Method or use according to any one of the preceding claims which further comprises contacting the identified modulator of CD28 with (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of CD28 or the fragment, to determine whether or not the modulator is capable of binding, or modulating the activity of, CD28.
    - 10. A crystal as defined in any one of claims 1, 7 or 8.

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- 11. Method of making a crystal as defined in any one of claims 1, 7 or 8 comprising providing a solution that comprises (i) CD28, (ii) a fragment of CD28, or (iii) a homologue of (i) or (ii), and optionally a CD28 specific antibody or fragment of said antibody, and subjecting the solution to conditions that cause the crystal to form.
  - 12. Method according to claim 11 comprising:
- (a) expressing (i), (ii) or (iii) in the form of a fusion protein with a second protein that is able to form a homodimer, wherein the presence of the second protein in the fusion protein causes (i), (ii) or (iii) to dimerise,
  - (b) cleaving the second protein from the fusion protein,
- (c) reducing and alkylating one or more of the disulphide bonds present in the stalk-like region of (i), (ii) or (iii), and
  - (d) crystallising (i), (ii) or (iii) bound to a Fab fragment of an antibody.

- Method according to 12 wherein the second protein mentioned in step (b) is an Fc fragment of an antibody.
- 14. Method according to any one of claims 11 to 13 wherein prior to crystallisation (i), (ii) or (iii) is expressed in the form of a fusion protein with an Fc fragment of an antibody, and optionally (i), (ii) or (iii) is cleaved from the fusion protein by thrombin.
- 15. Method according to any one of claims 11 to 14 wherein the (i), (ii) or (iii) is present in monomeric form in the crystal and/or one or more cysteine residues in the stalk-like region of (i), (ii) or (iii) are ethylated in the crystal.
- 16. A machine-readable data storage medium comprising a data storage material encoded with a machine readable data which when read by an appropriate machine is capable of displaying a representation of a crystal as defined in claim 1, 7 or 8.
  - 17. A computer program comprising program code means for performing the method or use of any one of claims 1 to 9 when said program is run on a computer.

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- 18. A computer program product comprising program code means stored on a computer readable storage medium for performing the method or use of any one of claims 1 to 9 when the said program product is run on a computer.
- 25 19. An antibody that induces superagonistic signalling by a cell surface receptor, wherein said antibody binds to the extracellular portion of the receptor at a membrane proximal region and said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase, wherein said antibody does not bind only the C'-D loop of human CD28.
  - 20. A chimeric protein that induces superagonistic signalling by a cell surface receptor, which chimeric protein comprises

- (i) sequence representing a fragment of a ligand of the receptor, or a homologue of such a fragment, wherein the fragment or homologue is capable of binding to the extracellular portion of the receptor at a membrane proximal region, and
- (ii) an Fc region of an antibody,
- wherein said receptor comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase.
  - 21. A chimeric protein that induces superagonistic signalling by one or two types of cell surface receptor, which chimeric protein comprises two Fv regions of an antibody that may be the same or different, wherein at least one of the Fv regions is capable of binding to a first receptor, and the other Fv region either binds to (i) said first receptor, or (ii) a second type of cell surface receptor which is found on a cell that contacts a cell which expresses (i), wherein said first receptor, and optionally also said second receptor, comprises a cytoplasmic domain which is dependent on an extrinsic protein kinase.
  - 22. An antibody or chimeric protein according to any one of claims 19 to 21 which
  - (i) binds orthogonally to the main axis of the domain of the receptor which it is binding, and/or
  - (ii) which lies parallel to the cell surface when bound to the receptor, and/or
  - (iii) which binds to a β-strand polypeptide chain of the receptor, and/or
  - (iv) which binds within 75Å of the cell surface.
- 23. An antibody or chimeric protein according to any one of claims 19 to 22 which binds to a sequence as shown in Table 1 or an equivalent homologous sequence in the proximal membrane region of a receptor which is capable of being induced to signal by the antibody or chimeric protein.
  - 24. An antibody or chimeric protein according to any one of claims 19 to 23 wherein said receptor
    - (i) comprises an ITAM motif, ITIM motif or "switch" signalling motif, and/or

- (ii) is a member of the CD28 family of proteins, and/or
- (iii) is expressed on the surface of a cell of the immune system, and/or
- (iv) comprises a cytoplasmic domain capable of being phosphorylated by a Src kinase, and/or
- (v) comprises a cytoplasmic domain capable of being dephosphorylated by CD45, and/or
  - (vi) is one of the receptors listed in Table 2, or is a homologue thereof.
  - 25. Method of obtaining an agent capable of inducing superagonistic signalling by a receptor as defined in claim 20 or 24, comprising determining whether a candidate agent binds to a membrane proximal extracellular region of the receptor, to thereby determine whether the candidate agent is capable of superagonising the receptor.
  - 26. Method according to claim 25 comprising determining whether a candidate agent which binds to the receptor, fails to bind to a mutated version of the receptor wherein one or more amino acids in a membrane proximal extracellular region of the receptor have been mutated, failure to bind to the mutant receptor indicating that the agent is capable of inducing superagonistic signalling by the receptor.
  - 27. Method according to claim 25 or 26 wherein the method is performed by contacting the candidate agent with (i) a full length receptor with said mutations, or (ii) a homologue of (i) with said mutations, or (iii) a fragment of (i) or (ii) comprising said mutations.
  - 28. Method according to claim 25 wherein the location of the binding of the candidate agent is determined by contacting the candidate agent with a peptide which comprises sequence from a membrane proximal extracellular region of the receptor and determining whether the candidate agent binds to the peptide, the binding of the candidate agent to a peptide indicating that the agent is capable of inducing superagonistic signalling by the receptor, wherein said sequence is at least 5 amino acids in length.

- 29. Method according to claim 28 comprising contacting the candidate agent with an array of overlapping peptides, which peptides represent fragments of the receptor and are 5 to 20 amino acids in length, the binding of the candidate agent to a peptide which represents a membrane proximal extracellular region of the receptor indicating that the agent is capable of inducing superagonistic signalling by the receptor.
- 30. Method of obtaining a superagonistic antibody as defined in any one of claims 19 or 22 to 24 comprising
- (i) screening antibodies for the ability to induce superagonistic signalling by a receptor according to claim 20 or 24, wherein said antibodies have been obtained by immunizing an animal with (a) said receptor, (b) a homologue of said receptor, or (c) a fragment of (a) or (b), or
  - (ii) screening antibodies for the ability to induce superagonistic signalling by a receptor according to claim 20 or 24, wherein said antibodies have been generated in a combinatorial antibody library.
  - 31. Method of obtaining a superagonistic antibody as defined in any one of claims 19 or 22 to 24 comprising
- (i) immunising an animal with a peptide comprising a sequence of length 5 to 20 amino acids which represents an extracellular membrane proximal region of the receptor and obtaining the antibody produced by the animal against said sequence, or (ii) selecting an antibody from a combinatorial antibody library based on its ability to bind a peptide as defined in (i), and optionally
- 25 (iii) recombinantly expressing the antibody obtained in (i) or (ii).

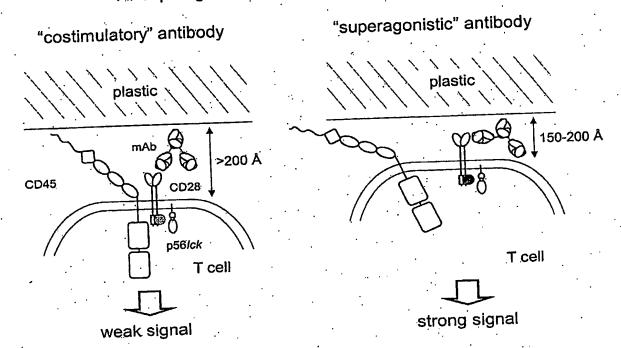
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- 32. Method according to any one of claims 1 to 9 or 25 to 31 further comprising formulating the identified modulator, obtained antibody or obtained agent into a pharmaceutical composition.
- 33. A peptide of length 5 to 20 amino acids comprising a sequence that binds to an antibody according to any one of claims 19 or 22 to 24.

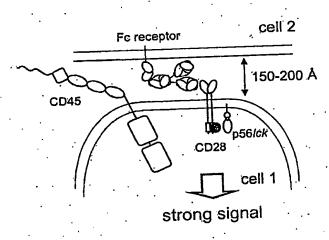
- 34. Method of inducing superagonistic signalling by a receptor according to claim 20 or 24 on a cell surface comprising sterically inhibiting contact between a phosphatase of the cell and the receptor, excluding a method in which an antibody that binds only the C'-D loop of CD28 is used to sterically inhibit contact between CD28 and the phosphatase CD45.
- 35. Method of modulating the immune response of a patient comprising administering to the patient:
- (i) a modulator identified by the method of any one of claims 1 to 9, or
  (ii) an antibody or chimeric protein according to any one of claims 19 to 24 or which is obtained by the method of claim 30 or 31; or
  - (iii) an agent obtained by the method of any one of claims 25 to 29, or
  - (iv) a peptide that stimulates an antibody response in the patient, wherein the antibody response comprises an antibody according to any one of claims 19 or 22 to
  - (vii) a nucleic acid capable of expressing (i), (ii), (iii) or (iv).

Figure 1

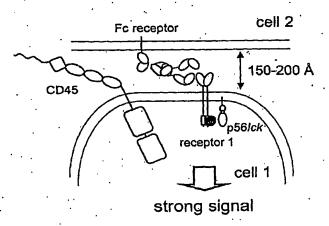
# A. Superagonistic antibody signalling in vitro



# B. Superagonistic antibody signalling in vivo



C. Chimeric protein 1 (ligand-based)

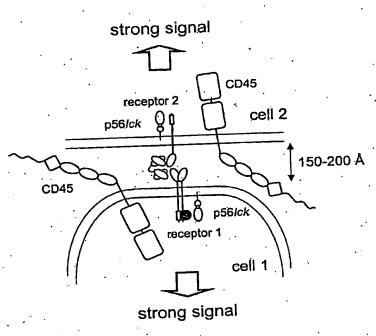




chimeric ligand/Fc superagonist:

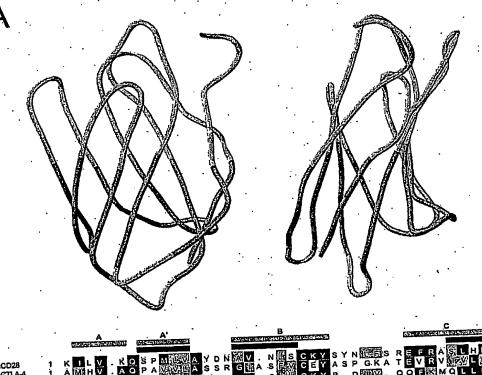
• binds Fc receptor on cell 1
and receptor 2 on cell 2

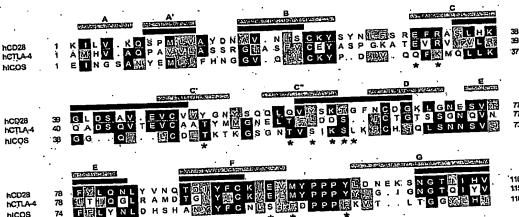
## D. Chimeric protein 2 (Fv-based)

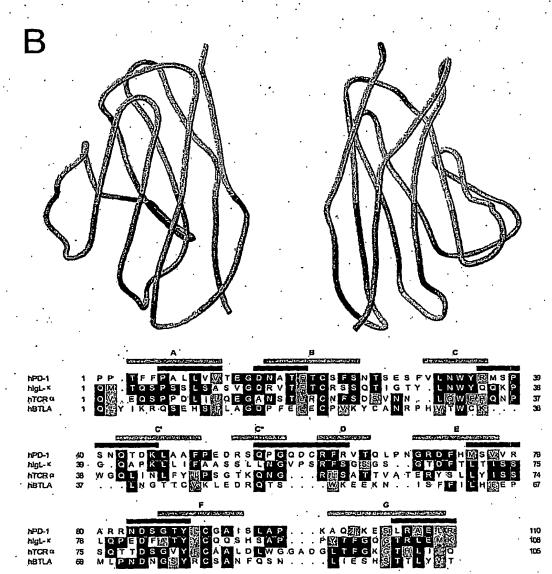


chimeric Fv superagonist:

• binds receptor 1 on cell 1 and receptor 2 on cell 2

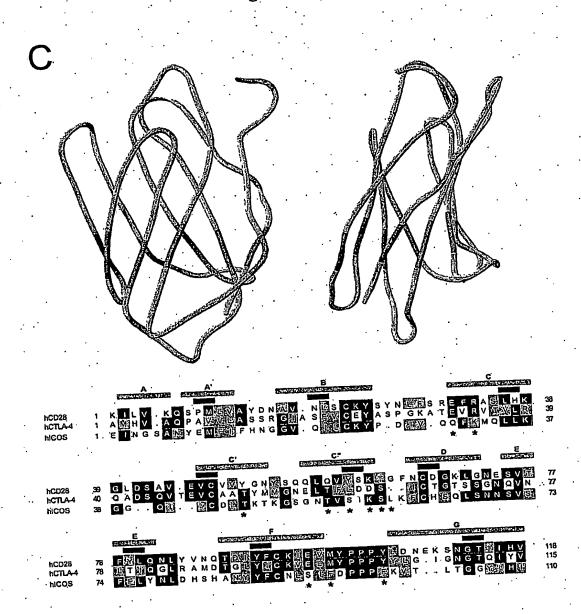






Docket/App No.: 3642.1000-000 Title: Receptor Modulators

Inventor: Simon Davis



hPD-1 higL-x hTCR a

